Computing with variational forms

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PRELIMINARY VERSION

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1 Basic principles for approximating differential equations

The finite element method is a very flexible approach for solving partial differential equations. Its two most attractive features are the ease of handling domains of complex shape in two and three dimensions and the ease of constructing higher-order discretization methods. The finite element method is usually applied for discretization in space, and therefore spatial problems will be our focus in the coming sections. Extensions to time-dependent problems may, for instance, use finite difference approximations in time.

Before studying how finite element methods are used to tackle differential equation, we first look at how global basis functions and the least squares, Galerkin, and collocation principles can be used to solve differential equations.

1.1 Differential equation models

Let us consider an abstract differential equation for a function $u(x)$ of one variable, written as

$$\mathcal{L}(u) = 0, \quad x \in \Omega\,. \tag{1}$$

Here are a few examples on possible choices of $\mathcal{L}(u)$, of increasing complexity:

$$\mathcal{L}(u) = \frac{d^2u}{dx^2} - f(x), \tag{2}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) + f(x), \tag{3}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) - au + f(x), \tag{4}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) + f(u,x)\,. \tag{5}$$

Both $\alpha(x)$ and $f(x)$ are considered as specified functions, while a is a prescribed parameter. Differential equations corresponding to (2)-(3) arise in diffusion phenomena, such as steady transport of heat in solids and flow of viscous fluids between flat plates. The form (4) arises when transient diffusion or wave phenomenon are discretized in time by finite differences. The equation (5) appear in chemical models when diffusion of a substance is combined with chemical reactions. Also in biology, (5) plays an important role, both for spreading of species and in models involving generation and propagation of electrical signals.

Let $\Omega = [0, L]$ be the domain in one space dimension. In addition to the differential equation, u must fulfill boundary conditions at the boundaries of the domain, $x = 0$ and $x = L$. When $\mathcal{L}$ contains up to second-order derivatives, as in the examples above, $m = 1$, we need one boundary condition at each of the (two) boundary points, here abstractly specified as

$$\mathcal{B}_0(u) = 0,\ x = 0, \quad \mathcal{B}_1(u) = 0,\ x = L \tag{6}$$

There are three common choices of boundary conditions:

$$\mathcal{B}_i(u) = u - g, \qquad \text{Dirichlet condition} \tag{7}$$

$$\mathcal{B}_i(u) = -\alpha\frac{du}{dx} - g, \qquad \text{Neumann condition} \tag{8}$$

$$\mathcal{B}_i(u) = -\alpha\frac{du}{dx} - h(u - g), \qquad \text{Robin condition} \tag{9}$$

Here, g and a are specified quantities.

From now on we shall use $u_{\mathrm{e}}(x)$ as symbol for the *exact* solution, fulfilling

$$\mathcal{L}(u_{\mathrm{e}}) = 0, \quad x \in \Omega, \tag{10}$$

while $u(x)$ is our notation for an *approximate* solution of the differential equation.

Remark on notation.

In the literature about the finite element method, is common to use u as the exact solution and u_h as the approximate solution, where h is a discretization parameter. However, the vast part of the present text is about the approximate solutions, and having a subscript h attached all the time is cumbersome. Of equal importance is the close correspondence between implementation and mathematics that we strive to achieve in this text: when it is natural to use `u` and not `u_h` in code, we let the mathematical notation be dictated by the code's preferred notation. After all, it is the powerful computer implementations of the finite element method that justifies studying the mathematical formulation and aspects of the method.

1.2 Simple model problems

A common model problem used much in the forthcoming examples is

$$-u''(x) = f(x), \quad x \in \Omega = [0, L], \quad u(0) = 0,\ u(L) = D\,. \tag{11}$$

A closely related problem with a different boundary condition at $x = 0$ reads

$$-u''(x) = f(x), \quad x \in \Omega = [0, L], \quad u'(0) = C,\ u(L) = D\,. \tag{12}$$

A third variant has a variable coefficient,

$$-(\alpha(x)u'(x))' = f(x), \quad x \in \Omega = [0, L], \quad u'(0) = C,\ u(L) = D\,. \tag{13}$$

We can easily solve these using `sympy`. For (11) we can write the function

```
def model1(f, L, D):
    """Solve -u'' = f(x), u(0)=0, u(L)=D."""
    u_x = - sp.integrate(f, (x, 0, x)) + c_0
    u = sp.integrate(u_x, (x, 0, x)) + c_1
    r = sp.solve([u.subs(x, 0)-0, u.subs(x,L)-D], [c_0, c_1])
    u = u.subs(c_0, r[c_0]).subs(c_1, r[c_1])
    u = sp.simplify(sp.expand(u))
    return u
```

Calling `model1(2, L, D)` results in the solution

$$u(x) = \frac{1}{L}x\left(D + L^2 - Lx\right) \tag{14}$$

Model (12) can be solved by


```
def model2(f, L, C, D):
    """Solve -u'' = f(x), u'(0)=C, u(L)=D."""
    u_x = - sp.integrate(f, (x, 0, x)) + c_0
    u = sp.integrate(u_x, (x, 0, x)) + c_1
    r = sp.solve([sp.diff(u,x).subs(x, 0)-C, u.subs(x,L)-D], [c_0, c_1])
    u = u.subs(c_0, r[c_0]).subs(c_1, r[c_1])
    u = sp.simplify(sp.expand(u))
    return u
```

to yield

$$u(x) = -x^2 + Cx - CL + D + L^2, \tag{15}$$

if $f(x) = 2$. Model (13) requires a bit more involved code,

```
def model3(f, a, L, C, D):
    """Solve -(a*u')' = f(x), u(0)=C, u(L)=D."""
    au_x = - sp.integrate(f, (x, 0, x)) + c_0
    u = sp.integrate(au_x/a, (x, 0, x)) + c_1
    r = sp.solve([u.subs(x, 0)-C, u.subs(x,L)-D], [c_0, c_1])
    u = u.subs(c_0, r[c_0]).subs(c_1, r[c_1])
    u = sp.simplify(sp.expand(u))
    return u
```

With $f(x) = 0$ and $\alpha(x) = 1 + x^2$ we get

$$u(x) = \frac{C\,\mathrm{atan}\,(L) - C\,\mathrm{atan}\,(x) + D\,\mathrm{atan}\,(x)}{\mathrm{atan}\,(L)}$$

1.3 Forming the residual

The fundamental idea is to seek an approximate solution u in some space V,

$$V = \mathrm{span}\{\psi_0(x), \ldots, \psi_N(x)\},$$

which means that u can always be expressed as a linear combination of the basis functions $\{\varphi_i\}_{i\in\mathcal{I}_s}$, with $\mathcal{I}_s$ as the index set $\{0, \ldots, N\}$:

$$u(x) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\,.$$

The coefficients $\{c_i\}_{i\in\mathcal{I}_s}$ are unknowns to be computed.

(Later, in Section 4, we will see that if we specify boundary values of u different from zero, we must look for an approximate solution $u(x) = B(x) + \sum_j c_j\psi_j(x)$, where $\sum_j c_j\psi_j \in V$ and $B(x)$ is some function for incorporating the right boundary values. Because of $B(x)$, u will not necessarily lie in V. This modification does not imply any difficulties.)

We need principles for deriving $N + 1$ equations to determine the $N + 1$ unknowns $\{c_i\}_{i\in\mathcal{I}_s}$. When approximating a given function f by $u = \sum_j c_j\varphi_j$, a key idea is to minimize the square norm of the approximation error $e = u - f$ or (equivalently) demand that e is orthogonal to V. Working with e is not so useful here since the approximation error in our case is $e = u_{\mathrm{e}} - u$ and u_{e} is unknown. The only general indicator we have on the quality of the approximate solution is to what degree u fulfills the differential equation. Inserting $u = \sum_j c_j\psi_j$ into $\mathcal{L}(u)$ reveals that the result is not zero, because u is only likely to equal u_{e}. The nonzero result,

$$R = \mathcal{L}(u) = \mathcal{L}(\sum_j c_j\psi_j), \tag{16}$$

is called the *residual* and measures the error in fulfilling the governing equation.

Various principles for determining $\{c_i\}_{i\in\mathcal{I}_s}$ try to minimize R in some sense. Note that R varies with x and the $\{c_i\}_{i\in\mathcal{I}_s}$ parameters. We may write this dependence explicitly as

$$R = R(x; c_0, \ldots, c_N)\,. \tag{17}$$

Below, we present three principles for making R small: a least squares method, a projection or Galerkin method, and a collocation or interpolation method.

1.4 The least squares method

The least-squares method aims to find $\{c_i\}_{i\in\mathcal{I}_s}$ such that the square norm of the residual

$$||R|| = (R, R) = \int_\Omega R^2 \,\mathrm{d}x \tag{18}$$

is minimized. By introducing an inner product of two functions f and g on Ω as

$$(f, g) = \int_\Omega f(x)g(x)\,\mathrm{d}x, \tag{19}$$

the least-squares method can be defined as

$$\min_{c_0,\ldots,c_N} E = (R, R)\,. \tag{20}$$

Differentiating with respect to the free parameters $\{c_i\}_{i\in\mathcal{I}_s}$ gives the $N+1$ equations

$$\int_\Omega 2R\frac{\partial R}{\partial c_i}\,\mathrm{d}x = 0 \quad \Leftrightarrow \quad (R, \frac{\partial R}{\partial c_i}) = 0, \quad i \in \mathcal{I}_s\,. \tag{21}$$

1.5 The Galerkin method

The least-squares principle is equivalent to demanding the error to be orthogonal to the space V when approximating a function f by $u \in V$. With a differential equation we do not know the true error so we must instead require the residual R to be orthogonal to V. This idea implies seeking $\{c_i\}_{i\in\mathcal{I}_s}$ such that

$$(R, v) = 0, \quad \forall v \in V\,. \tag{22}$$

This is the Galerkin method for differential equations.

This statement is equivalent to R being orthogonal to the $N+1$ basis functions only:

$$(R, \psi_i) = 0, \quad i \in \mathcal{I}_s, \tag{23}$$

resulting in $N+1$ equations for determining $\{c_i\}_{i\in\mathcal{I}_s}$.

1.6 The Method of Weighted Residuals

A generalization of the Galerkin method is to demand that R is orthogonal to some space W, but not necessarily the same space as V where we seek the unknown function. This generalization is naturally called the *method of weighted residuals*:

$$(R, v) = 0, \quad \forall v \in W\,. \tag{24}$$

If $\{w_0, \ldots, w_N\}$ is a basis for W, we can equivalently express the method of weighted residuals as

$$(R, w_i) = 0, \quad i \in \mathcal{I}_s\,. \tag{25}$$

The result is $N+1$ equations for $\{c_i\}_{i\in\mathcal{I}_s}$.

The least-squares method can also be viewed as a weighted residual method with $w_i = \partial R/\partial c_i$.

Variational formulation of the continuous problem.

Formulations like (24) (or (25)) and (22) (or (23)) are known as *variational formulations*. These equations are in this text primarily used for a numerical approximation $u \in V$, where V is a *finite-dimensional* space with dimension $N+1$. However, we may also let V be an *infinite-dimensional* space containing the exact solution $u_{\mathrm{e}}(x)$ such that also u_{e} fulfills the same variational formulation. The variational formulation is in that case a mathematical way of stating the problem and acts as an alternative to the usual formulation of a differential equation with initial and/or boundary conditions.

1.7 Test and Trial Functions

In the context of the Galerkin method and the method of weighted residuals it is common to use the name *trial function* for the approximate $u = \sum_j c_j\psi_j$. The space containing the trial function is known as the *trial space*. The function v entering the orthogonality requirement in the Galerkin method and the method of weighted residuals is called *test function*, and so are the ψ_i or w_i functions that are used as weights in the inner products with the residual. The space where the test functions comes from is naturally called the *test space*.

We see that in the method of weighted residuals the test and trial spaces are different and so are the test and trial functions. In the Galerkin method the test and trial spaces are the same (so far).

Remark.

It may be subject to debate whether it is only the form of (24) or (22) after integration by parts, as explained in Section 1.10, that qualifies for the term variational formulation. The result after integration by parts is what is obtained after taking the *first variation* of an optimization problem, see Section 1.13. However, here we use variational formulation as a common term for formulations which, in contrast to the differential equation $R = 0$, instead demand that an average of R is zero: $(R, v) = 0$ for all v in some space.

1.8 The collocation method

The idea of the collocation method is to demand that R vanishes at $N+1$ selected points $x_0, \ldots, x_N$ in Ω:

$$R(x_i; c_0, \ldots, c_N) = 0, \quad i \in \mathcal{I}_s\,. \tag{26}$$

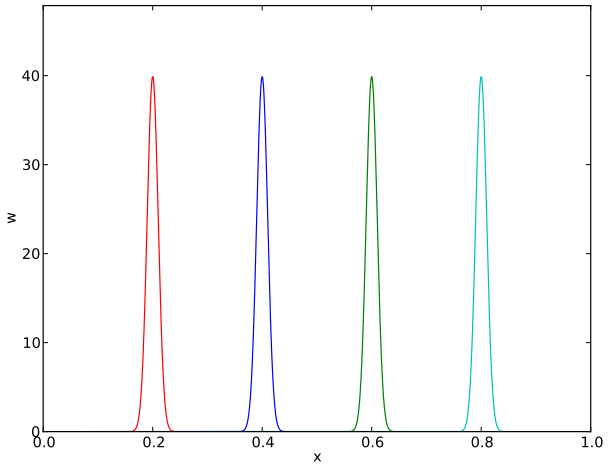


Figure 1: Approximation of delta functions by narrow Gaussian functions.

The collocation method can also be viewed as a method of weighted residuals with Dirac delta functions as weighting functions. Let $\delta(x-x_i)$ be the Dirac delta function centered around $x=x_i$ with the properties that $\delta(x-x_i)=0$ for $x\neq x_i$ and

$$\int_\Omega f(x)\delta(x-x_i)\,\mathrm{d}x = f(x_i), \quad x_i\in\Omega\,. \tag{27}$$

Intuitively, we may think of $\delta(x-x_i)$ as a very peak-shaped function around $x=x_i$ with integral 1, roughly visualized in Figure 1. Because of (27), we can let $w_i=\delta(x-x_i)$ be weighting functions in the method of weighted residuals, and (25) becomes equivalent to (26).

The subdomain collocation method. The idea of this approach is to demand the integral of R to vanish over $N+1$ subdomains Ω_i of Ω:

$$\int_{\Omega_i} R\,\mathrm{d}x = 0, \quad i\in\mathcal{I}_s\,. \tag{28}$$

This statement can also be expressed as a weighted residual method

$$\int_\Omega Rw_i\,\mathrm{d}x = 0, \quad i\in\mathcal{I}_s, \tag{29}$$

where $w_i=1$ for $x\in\Omega_i$ and $w_i=0$ otherwise.

1.9 Examples on using the principles

Let us now apply global basis functions to illustrate the principles for minimizing R.

The model problem. We consider the differential equation problem

$$-u''(x)=f(x), \quad x\in\Omega=[0,L], \quad u(0)=0,\ u(L)=0\,. \tag{30}$$

Basis functions. Our choice of basis functions ψ_i for V is

$$\psi_i(x)=\sin\left((i+1)\pi\frac{x}{L}\right), \quad i\in\mathcal{I}_s\,. \tag{31}$$

An important property of these functions is that $\psi_i(0)=\psi_i(L)=0$, which means that the boundary conditions on u are fulfilled:

$$u(0)=\sum_j c_j\psi_j(0)=0, \quad u(L)=\sum_j c_j\psi_j(L)=0\,.$$

Another nice property is that the chosen sine functions are orthogonal on Ω:

$$\int_0^L \sin\left((i+1)\pi\frac{x}{L}\right)\sin\left((j+1)\pi\frac{x}{L}\right)\,\mathrm{d}x = \begin{cases} \frac{1}{2}L & i=j \\ 0, & i\neq j \end{cases} \tag{32}$$

provided i and j are integers.

The residual. We can readily calculate the following explicit expression for the residual:

$$\begin{aligned} R(x;c_0,\ldots,c_N) &= u''(x)+f(x), \\ &= \frac{d^2}{dx^2}\left(\sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\right)+f(x), \\ &= \sum_{j\in\mathcal{I}_s} c_j\psi_j''(x)+f(x)\,. \end{aligned} \tag{33}$$

The least squares method. The equations (21) in the least squares method require an expression for $\partial R/\partial c_i$. We have

$$\frac{\partial R}{\partial c_i}=\frac{\partial}{\partial c_i}\left(\sum_{j\in\mathcal{I}_s} c_j\psi_j''(x)+f(x)\right)=\sum_{j\in\mathcal{I}_s}\frac{\partial c_j}{\partial c_i}\psi_j''(x)=\psi_i''(x)\,. \tag{34}$$

The governing equations for $\{c_i\}_{i\in\mathcal{I}_s}$ are then

$$(\sum_j c_j\psi_j''+f,\psi_i'')=0, \quad i\in\mathcal{I}_s, \tag{35}$$

which can be rearranged as

$$\sum_{j\in\mathcal{I}_s}(\psi_i'',\psi_j'')c_j=-(f,\psi_i''), \quad i\in\mathcal{I}_s\,. \tag{36}$$

This is nothing but a linear system

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i, \quad i \in \mathcal{I}_s,$$

with

$$\begin{aligned} A_{i,j} &= (\psi_i'', \psi_j'') \\ &= \pi^4(i+1)^2(j+1)^2L^{-4}\int_0^L \sin\left((i+1)\pi\frac{x}{L}\right)\sin\left((j+1)\pi\frac{x}{L}\right)\,\mathrm{d}x \\ &= \begin{cases} \frac{1}{2}L^{-3}\pi^4(i+1)^4 & i=j \\ 0, & i\neq j \end{cases} \end{aligned} \tag{37}$$

$$b_i = -(f,\psi_i'') = (i+1)^2\pi^2L^{-2}\int_0^L f(x)\sin\left((i+1)\pi\frac{x}{L}\right)\,\mathrm{d}x \tag{38}$$

Since the coefficient matrix is diagonal we can easily solve for

$$c_i = \frac{2L}{\pi^2(i+1)^2}\int_0^L f(x)\sin\left((i+1)\pi\frac{x}{L}\right)\,\mathrm{d}x\,. \tag{39}$$

With the special choice of $f(x) = 2$ can be calculated in `sympy` by

```
from sympy import *
import sys

i, j = symbols('i j', integer=True)
x, L = symbols('x L')
f = 2
a = 2*L/(pi**2*(i+1)**2)
c_i = a*integrate(f*sin((i+1)*pi*x/L), (x, 0, L))
c_i = simplify(c_i)
print c_i
```

The answer becomes

$$c_i = 4\frac{L^2\left((-1)^i+1\right)}{\pi^3\left(i^3+3i^2+3i+1\right)}$$

Now, $1+(-1)^i = 0$ for i odd, so only the coefficients with even index are nonzero. Introducing $i = 2k$ for $k = 0,\ldots,N/2$ to count the relevant indices (for N odd, k goes to $(N-1)/2$), we get the solution

$$u(x) = \sum_{k=0}^{N/2}\frac{8L^2}{\pi^3(2k+1)^3}\sin\left((2k+1)\pi\frac{x}{L}\right)\,. \tag{40}$$

The coefficients decay very fast: $c_2 = c_0/27$, $c_4 = c_0/125$. The solution will therefore be dominated by the first term,

$$u(x) \approx \frac{8L^2}{\pi^3}\sin\left(\pi\frac{x}{L}\right)\,.$$

The Galerkin method. The Galerkin principle (22) applied to (30) consists of inserting our special residual (33) in (22)

$$(u''+f, v) = 0, \quad \forall v \in V,$$

or

$$(u'', v) = -(f, v), \quad \forall v \in V\,. \tag{41}$$

This is the variational formulation, based on the Galerkin principle, of our differential equation. The $\forall v \in V$ requirement is equivalent to demanding the equation $(u'', v) = -(f, v)$ to be fulfilled for all basis functions $v = \psi_i$, $i \in \mathcal{I}_s$, see (22) and (23). We therefore have

$$(\sum_{j\in\mathcal{I}_s} c_j\psi_j'', \psi_i) = -(f,\psi_i), \quad i \in \mathcal{I}_s\,. \tag{42}$$

This equation can be rearranged to a form that explicitly shows that we get a linear system for the unknowns $\{c_i\}_{i\in\mathcal{I}_s}$:

$$\sum_{j\in\mathcal{I}_s}(\psi_i, \psi_j'')c_j = (f,\psi_i), \quad i \in \mathcal{I}_s\,. \tag{43}$$

For the particular choice of the basis functions (31) we get in fact the same linear system as in the least squares method because $\psi'' = -(i+1)^2\pi^2L^{-2}\psi$.

The collocation method. For the collocation method (26) we need to decide upon a set of $N+1$ collocation points in Ω. A simple choice is to use uniformly spaced points: $x_i = i\Delta x$, where $\Delta x = L/N$ in our case ($N \geq 1$). However, these points lead to at least two rows in the matrix consisting of zeros (since $\psi_i(x_0) = 0$ and $\psi_i(x_N) = 0$), thereby making the matrix singular and non-invertible. This forces us to choose some other collocation points, e.g., random points or points uniformly distributed in the interior of Ω. Demanding the residual to vanish at these points leads, in our model problem (30), to the equations

$$-\sum_{j\in\mathcal{I}_s} c_j\psi_j''(x_i) = f(x_i), \quad i \in \mathcal{I}_s, \tag{44}$$

which is seen to be a linear system with entries

$$A_{i,j} = -\psi_j''(x_i) = (j+1)^2\pi^2L^{-2}\sin\left((j+1)\pi\frac{x_i}{L}\right),$$

in the coefficient matrix and entries $b_i = 2$ for the right-hand side (when $f(x) = 2$).

The special case of $N = 0$ can sometimes be of interest. A natural choice is then the midpoint $x_0 = L/2$ of the domain, resulting in $A_{0,0} = -\psi_0''(x_0) = \pi^2L^{-2}$, $f(x_0) = 2$, and hence $c_0 = 2L^2/\pi^2$.

Comparison. In the present model problem, with $f(x) = 2$, the exact solution is $u(x) = x(L-x)$, while for $N = 0$ the Galerkin and least squares method result in $u(x) = 8L^2\pi^{-3}\sin(\pi x/L)$ and the collocation method leads to $u(x) = 2L^2\pi^{-2}\sin(\pi x/L)$. We can quickly use `sympy` to verify that the maximum error occurs at the midpoint $x = L/2$ and find what the errors are:

```
>>> import sympy as sp
>>> # Computing with Dirichlet conditions: -u''=2 and sines
>>> x, L = sp.symbols('x L')
>>> e_Galerkin = x*(L-x) - 8*L**2*sp.pi**(-3)*sp.sin(sp.pi*x/L)
>>> e_colloc = x*(L-x) - 2*L**2*sp.pi**(-2)*sp.sin(sp.pi*x/L)

>>> # Verify max error for x=L/2
>>> dedx_Galerkin = sp.diff(e_Galerkin, x)
>>> dedx_Galerkin.subs(x, L/2)
0
>>> dedx_colloc = sp.diff(e_colloc, x)
>>> dedx_colloc.subs(x, L/2)
0

# Compute max error: x=L/2, evaluate numerical, and simplify
>>> sp.simplify(e_Galerkin.subs(x, L/2).evalf(n=3))
-0.00812*L**2
>>> sp.simplify(e_colloc.subs(x, L/2).evalf(n=3))
0.0473*L**2
```

The error in the collocation method is about 6 times larger than the error in the Galerkin or least squares method.

1.10 Integration by parts

A problem arises if we want to apply popular finite element functions to solve our model problem (30) by the standard least squares, Galerkin, or collocation methods: the piecewise polynomials $\psi_i(x)$ have discontinuous derivatives at the cell boundaries which makes it problematic to compute the second-order derivative. This fact actually makes the least squares and collocation methods less suitable for finite element approximation of the unknown function. (By rewriting the equation $-u'' = f$ as a system of two first-order equations, $u' = v$ and $-v' = f$, the least squares method can be applied. Also, differentiating discontinuous functions can actually be handled by distribution theory in mathematics.) The Galerkin method and the method of weighted residuals can, however, be applied together with finite element basis functions if we use *integration by parts* as a means for transforming a second-order derivative to a first-order one.

Consider the model problem (30) and its Galerkin formulation

$$-(u'', v) = (f, v) \quad \forall v \in V\,.$$

Using integration by parts in the Galerkin method, we can move a derivative of u onto v:

$$\begin{aligned}\int_0^L u''(x)v(x)\,\mathrm{d}x &= -\int_0^L u'(x)v'(x)\,\mathrm{d}x + [vu']_0^L \\ &= -\int_0^L u'(x)v'(x)\,\mathrm{d}x + u'(L)v(L) - u'(0)v(0)\,. \end{aligned} \tag{45}$$

Usually, one integrates the problem at the stage where the u and v functions enter the formulation. Alternatively, but less common, we can integrate by parts in the expressions for the matrix entries:

$$\begin{aligned}\int_0^L \psi_i(x)\psi_j''(x)\,\mathrm{d}x &= -\int_0^L \psi_i'(x)\psi_j'(x)dx + [\psi_i\psi_j']_0^L \\ &= -\int_0^L \psi_i'(x)\psi_j'(x)\,\mathrm{d}x + \psi_i(L)\psi_j'(L) - \psi_i(0)\psi_j'(0)\,. \end{aligned} \tag{46}$$

Integration by parts serves to reduce the order of the derivatives and to make the coefficient matrix symmetric since $(\psi_i', \psi_j') = (\psi_i', \psi_j')$. The symmetry property depends on the type of terms that enter the differential equation. As will be seen later in Section 5, integration by parts also provides a method for implementing boundary conditions involving u'.

With the choice (31) of basis functions we see that the "boundary terms" $\psi_i(L)\psi_j'(L)$ and $\psi_i(0)\psi_j'(0)$ vanish since $\psi_i(0) = \psi_i(L) = 0$.

Weak form. Since the variational formulation after integration by parts make weaker demands on the differentiability of u and the basis functions ψ_i, the resulting integral formulation is referred to as a *weak form* of the differential equation problem. The original variational formulation with second-order derivatives, or the differential equation problem with second-order derivative, is then the *strong form*, with stronger requirements on the differentiability of the functions.

For differential equations with second-order derivatives, expressed as variational formulations and solved by finite element methods, we will always perform integration by parts to arrive at expressions involving only first-order derivatives.

1.11 Boundary function

So far we have assumed zero Dirichlet boundary conditions, typically $u(0) = u(L) = 0$, and we have demanded that $\psi_i(0) = \psi_i(L) = 0$ for $i \in \mathcal{I}_s$. What about a boundary condition like $u(L) = D \neq 0$? This condition immediately faces a problem: $u = \sum_j c_j\varphi_j(L) = 0$ since all $\varphi_i(L) = 0$.

A boundary condition of the form $u(L) = D$ can be implemented by demanding that all $\psi_i(L) = 0$, but adding a *boundary function* $B(x)$ with the right boundary value, $B(L) = D$, to the expansion for u:

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\,.$$

This u gets the right value at $x = L$:

$$u(L) = B(L) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(L) = B(L) = D\,.$$

The idea is that for any boundary where u is known we demand ψ_i to vanish and construct a function $B(x)$ to attain the boundary value of u. There are no restrictions how $B(x)$ varies with x in the interior of the domain, so this variation needs to be constructed in some way.

For example, with $u(0) = 0$ and $u(L) = D$, we can choose $B(x) = xD/L$, since this form ensures that $B(x)$ fulfills the boundary conditions: $B(0) = 0$ and $B(L) = D$. The unknown function is then sought on the form

$$u(x) = \frac{x}{L}D + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x), \tag{47}$$

with $\psi_i(0) = \psi_i(L) = 0$.

The $B(x)$ function can be chosen in many ways as long as its boundary values are correct. For example, $B(x) = D(x/L)^p$ for any power p will work fine in the above example.

As another example, consider a domain $\Omega = [a, b]$ where the boundary conditions are $u(a) = U_a$ and $u(b) = U_b$. A class of possible $B(x)$ functions is

$$B(x) = U_a + \frac{U_b - U_a}{(b-a)^p}(x-a)^p, \quad p > 0\,. \tag{48}$$

Real applications will most likely use the simplest version, $p = 1$, but here such a p parameter was included to demonstrate the ambiguity in the construction of $B(x)$.

Summary.

The general procedure of incorporating Dirichlet boundary conditions goes as follows. Let $\partial\Omega_E$ be the part(s) of the boundary $\partial\Omega$ of the domain Ω where u is specified. Set $\psi_i = 0$ at the points in $\partial\Omega_E$ and seek u as

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x), \tag{49}$$

where $B(x)$ equals the boundary conditions on u at $\partial\Omega_E$.

Remark. With the $B(x)$ term, u does not in general lie in $V = \text{span}\,\{\psi_0, \ldots, \psi_N\}$ anymore. Moreover, when a prescribed value of u at the boundary, say $u(a) = U_a$ is different from zero, it does not make sense to say that u lies in a vector space, because this space does not obey the requirements of addition and scalar multiplication. For example, $2u$ does not lie in the space since its boundary value is $2U_a$, which is incorrect. It only makes sense to split u in two parts, as done above, and have the unknown part $\sum_j c_j\psi_j$ in a proper function space.

1.12 Abstract notation for variational formulations

We have seen that variational formulations end up with a formula involving u and v, such as (u', v') and a formula involving v and known functions, such as (f, v). A widely used notation is to introduce an abstract variational statement written as $a(u, v) = L(v)$, where $a(u, v)$ is a so-called *bilinear form* involving all the terms that contain both the test and trial function, while $L(v)$ is a *linear form* containing all the terms without the trial function. For example, the statement

$$\int_\Omega u'v'\,\mathrm{d}x = \int_\Omega fv\,\mathrm{d}x \quad \text{or} \quad (u', v') = (f, v) \quad \forall v \in V$$

can be written in abstract form: *find u such that*

$$a(u, v) = L(v) \quad \forall v \in V,$$

where we have the definitions

$$a(u, v) = (u', v'), \quad L(v) = (f, v)\,.$$

The term *linear* means that $L(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 L(v_1) + \alpha_2 L(v_2)$ for two test functions v_1 and v_2, and scalar parameters α_1 and α_2. Similarly, the term *bilinear* means that $a(u, v)$ is linear in both its arguments:

$$a(\alpha_1 u_1 + \alpha_2 u_2, v) = \alpha_1 a(u_1, v) + \alpha_2 a(u_2, v),$$
$$a(u, \alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 a(u, v_1) + \alpha_2 a(u, v_2)\,.$$

In nonlinear problems these linearity properties do not hold in general and the abstract notation is then $F(u; v) = 0$.

The matrix system associated with $a(u, v) = L(v)$ can also be written in an abstract form by inserting $v = \psi_i$ and $u = \sum_j c_j\psi_j$ in $a(u, v) = L(v)$. Using the linear properties, we get

$$\sum_{j\in\mathcal{I}_s} a(\psi_j, \psi_i)c_j = L(\psi_i), \quad i \in \mathcal{I}_s,$$

which is a linear system

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i, \quad i \in \mathcal{I}_s,$$

where

$$A_{i,j} = a(\psi_j, \psi_i), \quad b_i = L(\psi_i)\,.$$

In many problems, $a(u, v)$ is symmetric such that $a(\psi_j, \psi_i) = a(\psi_i, \psi_j)$. In those cases the coefficient matrix becomes symmetric, $A_{i,j} = A_{j,i}$, a property that can simplify solution algorithms for linear systems and make them more stable in addition to saving memory and computations.

The abstract notation $a(u, v) = L(v)$ for linear differential equation problems is much used in the literature and in description of finite element software (in particular the FEniCS[1] documentation). We shall frequently summarize variational forms using this notation.

1.13 Variational problems and optimization of functionals

If $a(u, v) = a(v, u)$, it can be shown that the variational statement

$$a(u, v) = L(v) \quad \forall v \in V,$$

is equivalent to minimizing the functional

$$F(v) = \frac{1}{2}a(v, v) - L(v)$$

over all functions $v \in V$. That is,

$$F(u) \leq F(v) \quad \forall v \in V\,.$$

Inserting a $v = \sum_j c_j\psi_j$ turns minimization of $F(v)$ into minimization of a quadratic function

$$\bar{F}(c_0, \ldots, c_N) = \sum_{j\in\mathcal{I}_s}\sum_{i\in\mathcal{I}_s} a(\psi_i, \psi_j)c_ic_j - \sum_{j\in\mathcal{I}_s} L(\psi_j)c_j$$

of $N + 1$ parameters.

Minimization of $\bar{F}$ implies

$$\frac{\partial\bar{F}}{\partial c_i} = 0, \quad i \in \mathcal{I}_s\,.$$

After some algebra one finds

$$\sum_{j\in\mathcal{I}_s} a(\psi_i, \psi_j)c_j = L(\psi_i), \quad i \in \mathcal{I}_s,$$

which is the same system as that arising from $a(u, v) = L(v)$.

[1] `http://fenicsproject.org`

Many traditional applications of the finite element method, especially in solid mechanics and structural analysis, start with formulating $F(v)$ from physical principles, such as minimization of energy, and then proceeds with deriving $a(u,v) = L(v)$, which is the equation usually desired in implementations.

2 Examples on variational formulations

The following sections derive variational formulations for some prototype differential equations in 1D, and demonstrate how we with ease can handle variable coefficients, mixed Dirichlet and Neumann boundary conditions, first-order derivatives, and nonlinearities.

2.1 Variable coefficient

Consider the problem

$$-\frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) = f(x), \quad x\in\Omega=[0,L],\ u(0)=C,\ u(L)=D\,. \tag{50}$$

There are two new features of this problem compared with previous examples: a variable coefficient $a(x)$ and nonzero Dirichlet conditions at both boundary points.

Let us first deal with the boundary conditions. We seek

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_i(x),$$

with $\psi_i(0)=\psi_i(L)=0$ for $i\in\mathcal{I}_s$. The function $B(x)$ must then fulfill $B(0)=C$ and $B(L)=D$. How B varies in between $x=0$ and $x=L$ is not of importance. One possible choice is

$$B(x) = C + \frac{1}{L}(D-C)x,$$

which follows from (48) with $p=1$.

We seek $(u-B)\in V$. As usual,

$$V = \text{span}\{\psi_0,\ldots,\psi_N\},$$

but the two Dirichlet boundary conditions demand that

$$\psi_i(0)=\psi_i(L)=0, \quad i\in\mathcal{I}_s\,.$$

Note that any $v\in V$ has the property $v(0)=v(L)=0$.

The residual arises by inserting our u in the differential equation:

$$R = -\frac{d}{dx}\left(\alpha\frac{du}{dx}\right) - f\,.$$

Galerkin's method is

$$(R,v)=0, \quad \forall v\in V,$$

or written with explicit integrals,

$$\int_\Omega\left(-\frac{d}{dx}\left(\alpha\frac{du}{dx}\right) - f\right)v\,\mathrm{d}x = 0, \quad \forall v\in V\,.$$

We proceed with integration by parts to lower the derivative from second to first order:

$$-\int_\Omega\frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right)v\,\mathrm{d}x = \int_\Omega\alpha(x)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x - \left[\alpha\frac{du}{dx}v\right]_0^L\,.$$

The boundary term vanishes since $v(0)=v(L)=0$. The variational formulation is then

$$\int_\Omega\alpha(x)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x = \int_\Omega f(x)v\,\mathrm{d}x, \quad \forall v\in V\,.$$

The variational formulation can alternatively be written in a more compact form:

$$(\alpha u', v') = (f,v), \quad \forall v\in V\,.$$

The corresponding abstract notation reads

$$a(u,v) = L(v) \quad \forall v\in V,$$

with

$$a(u,v) = (\alpha u', v'), \quad L(v) = (f,v)\,.$$

Note that the a in the notation $a(\cdot,\cdot)$ is not to be mixed with the variable coefficient $a(x)$ in the differential equation.

We may insert $u = B + \sum_j c_j\psi_j$ and $v=\psi_i$ to derive the linear system:

$$(\alpha B' + \alpha\sum_{j\in\mathcal{I}_s} c_j\psi_j', \psi_i') = (f,\psi_i), \quad i\in\mathcal{I}_s\,.$$

Isolating everything with the c_j coefficients on the left-hand side and all known terms on the right-hand side gives

$$\sum_{j\in\mathcal{I}_s}(\alpha\psi_j',\psi_i')c_j = (f,\psi_i) + (a(D-C)L^{-1},\psi_i'), \quad i\in\mathcal{I}_s\,.$$

This is nothing but a linear system $\sum_j A_{i,j}c_j = b_i$ with

$$A_{i,j} = (a\psi_j',\psi_i') = \int_\Omega\alpha(x)\psi_j'(x),\psi_i'(x)\,\mathrm{d}x,$$
$$b_i = (f,\psi_i) + (a(D-C)L^{-1},\psi_i') = \int_\Omega\left(f(x)\psi_i(x) + \alpha(x)\frac{D-C}{L}\psi_i'(x)\right)\mathrm{d}x\,.$$

2.2 First-order derivative in the equation and boundary condition

The next problem to formulate in variational form reads

$$-u''(x) + bu'(x) = f(x), \quad x\in\Omega=[0,L],\ u(0)=C,\ u'(L)=E\,. \tag{51}$$

The new features are a first-order derivative u' in the equation and the boundary condition involving the derivative: $u'(L)=E$. Since we have a Dirichlet condition at $x=0$, we must force $\psi_i(0)=0$ and use a boundary function to take care of the condition $u(0)=C$. Because there is no Dirichlet condition on $x=L$ we do not make any requirements to $\psi_i(L)$. The simplest possible choice of $B(x)$ is $B(x)=C$.

The expansion for u becomes

$$u = C + \sum_{j\in\mathcal{I}_s} c_j\psi_i(x)\,.$$

The variational formulation arises from multiplying the equation by a test function $v \in V$ and integrating over Ω:

$$(-u'' + bu' - f, v) = 0, \quad \forall v \in V$$

We apply integration by parts to the $u''v$ term only. Although we could also integrate $u'v$ by parts, this is not common. The result becomes

$$(u', v') + (bu', v) = (f, v) + [u'v]_0^L, \quad \forall v \in V\,.$$

Now, $v(0) = 0$ so

$$[u'v]_0^L = u'(L)v(L) = Ev(L),$$

because $u'(L) = E$. Integration by parts allows us to take care of the Neumann condition in the boundary term.

Natural and essential boundary conditions.

Omitting a boundary term like $[u'v]_0^L$ implies that we actually impose the condition $u' = 0$ unless there is a Dirichlet condition (i.e., $v = 0$) at that point! This result has great practical consequences, because it is easy to forget the boundary term, and this mistake may implicitly set a boundary condition! Since homogeneous Neumann conditions can be incorporated without doing anything, and non-homogeneous Neumann conditions can just be inserted in the boundary term, such conditions are known as *natural boundary conditions*. Dirichlet conditions requires more essential steps in the mathematical formulation, such as forcing all $\varphi_i = 0$ on the boundary and constructing a $B(x)$, and are therefore known as *essential boundary conditions*.

The final variational form reads

$$(u', v') + (bu', v) = (f, v) + Ev(L), \quad \forall v \in V\,.$$

In the abstract notation we have

$$a(u, v) = L(v) \quad \forall v \in V,$$

with the particular formulas

$$a(u, v) = (u', v') + (bu', v), \quad L(v) = (f, v) + Ev(L)\,.$$

The associated linear system is derived by inserting $u = B + \sum_j c_j\psi_j$ and replacing v by ψ_i for $i \in \mathcal{I}_s$. Some algebra results in

$$\sum_{j\in\mathcal{I}_s} \underbrace{((\psi_j', \psi_i') + (b\psi_j', \psi_i))}_{A_{i,j}} c_j = \underbrace{(f, \psi_i) + E\psi_i(L)}_{b_i}\,.$$

Observe that in this problem, the coefficient matrix is not symmetric, because of the term

$$(b\psi_j', \psi_i) = \int_\Omega b\psi_j'\psi_i\,\mathrm{d}x \neq \int_\Omega b\psi_i'\psi_j\,\mathrm{d}x = (\psi_i', b\psi_j)\,.$$

2.3 Nonlinear coefficient

Finally, we show that the techniques used above to derive variational forms also apply to nonlinear differential equation problems as well. Here is a model problem with a nonlinear coefficient and right-hand side:

$$-(\alpha(u)u')' = f(u), \quad x \in [0, L],\ u(0) = 0,\ u'(L) = E\,. \tag{52}$$

Our space V has basis $\{\psi_i\}_{i\in\mathcal{I}_s}$, and because of the condition $u(0) = 0$, we must require $\psi_i(0) = 0$, $i \in \mathcal{I}_s$.

Galerkin's method is about inserting the approximate u, multiplying the differential equation by $v \in V$, and integrate,

$$-\int_0^L \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) v\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x \quad \forall v \in V\,.$$

The integration by parts does not differ from the case where we have $\alpha(x)$ instead of $\alpha(u)$:

$$\int_0^L \alpha(u)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x + [\alpha(u)vu']_0^L \quad \forall v \in V\,.$$

The term $\alpha(u(0))v(0)u'(0) = 0$ since $v(0)$. The other term, $\alpha(u(L))v(L)u'(L)$, is used to impose the other boundary condition $u'(L) = E$, resulting in

$$\int_0^L \alpha(u)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x + \alpha(u(L))v(L)E \quad \forall v \in V,$$

or alternatively written more compactly as

$$(\alpha(u)u', v') = (f(u), v) + \alpha(u(L))v(L)E \quad \forall v \in V\,.$$

Since the problem is nonlinear, we cannot identify a bilinear form $a(u, v)$ and a linear form $L(v)$. An abstract notation is typically *find u such that*

$$F(u; v) = 0 \quad \forall v \in V,$$

with

$$F(u; v) = (a(u)u', v') - (f(u), v) - a(L)v(L)E\,.$$

By inserting $u = \sum_j c_j\psi_j$ we get a *nonlinear system of algebraic equations* for the unknowns c_i, $i \in \mathcal{I}_s$. Such systems must be solved by constructing a sequence of linear systems whose solutions hopefully converge to the solution of the nonlinear system. Frequently applied methods are Picard iteration and Newton's method.

2.4 Computing with Dirichlet and Neumann conditions

Let us perform the necessary calculations to solve

$$-u''(x) = 2, \quad x \in \Omega = [0,1], \quad u'(0) = C,\ u(1) = D,$$

using a global polynomial basis $\psi_i \sim x^i$. The requirements on ψ_i is that $\psi_i(1) = 0$, because u is specified at $x = 1$, so a proper set of polynomial basis functions can be

$$\psi_i(x) = (1-x)^{i+1}, \quad i \in \mathcal{I}_s\,.$$

A suitable $B(x)$ function to handle the boundary condition $u(1) = D$ is $B(x) = Dx$. The variational formulation becomes

$$(u', v') = (2, v) - Cv(0) \quad \forall v \in V\,.$$

From inserting $u = B + \sum_j c_j\psi_j$ and choosing $v = \psi_i$ we get

$$\sum_{j\in\mathcal{I}_s} (\psi_j', \psi_i')c_j = (2, \psi_i) - (B', \psi_i') - C\psi_i(0), \quad i \in \mathcal{I}_s\,.$$

The entries in the linear system are then

$$\begin{aligned}
A_{i,j} &= (\psi_j', \psi_i') = \int_0^1 \psi_i'(x)\psi_j'(x)\,\mathrm{d}x = \int_0^1 (i+1)(j+1)(1-x)^{i+j}\,\mathrm{d}x = \frac{(i+1)(j+1)}{i+j+1},\\
b_i &= (2, \psi_i) - (D, \psi_i') - C\psi_i(0)\\
&= \int_0^1 \left(2\psi_i(x) - D\psi_i'(x)\right)\,\mathrm{d}x - C\psi_i(0)\\
&= \int_0^1 \left(2(1-x)^{i+1} - D(i+1)(1-x)^i\right)\,\mathrm{d}x - C\\
&= \frac{(D-C)(i+2)+2}{i+2} = D - C + \frac{2}{i+2}\,.
\end{aligned}$$

Relevant `sympy` commands to help calculate these expressions are

```
from sympy import *
x, C, D = symbols('x C D')
i, j = symbols('i j', integer=True, positive=True)
psi_i = (1-x)**(i+1)
psi_j = psi_i.subs(i, j)
integrand = diff(psi_i, x)*diff(psi_j, x)
integrand = simplify(integrand)
A_ij = integrate(integrand, (x, 0, 1))
A_ij = simplify(A_ij)
print 'A_ij:', A_ij
f = 2
b_i = integrate(f*psi_i, (x, 0, 1)) - \
      integrate(diff(D*x, x)*diff(psi_i, x), (x, 0, 1)) - \
      C*psi_i.subs(x, 0)
b_i = simplify(b_i)
print 'b_i:', b_i
```

The output becomes


```
A_ij: (i + 1)*(j + 1)/(i + j + 1)
b_i: ((-C + D)*(i + 2) + 2)/(i + 2)
```

We can now choose some N and form the linear system, say for $N = 1$:

```
N = 1
A = zeros((N+1, N+1))
b = zeros(N+1)
print 'fresh b:', b
for r in range(N+1):
    for s in range(N+1):
        A[r,s] = A_ij.subs(i, r).subs(j, s)
    b[r,0] = b_i.subs(i, r)
```

The system becomes

$$\begin{pmatrix} 1 & 1 \\ 1 & 4/3 \end{pmatrix}\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} 1 - C + D \\ 2/3 - C + D \end{pmatrix}$$

The solution (`c = A.LUsolve(b)`) becomes $c_0 = 2 - C + D$ and $c_1 = -1$, resulting in

$$u(x) = 1 - x^2 + D + C(x-1), \tag{53}$$

We can form this u in `sympy` and check that the differential equation and the boundary conditions are satisfied:

```
u = sum(c[r,0]*psi_i.subs(i, r) for r in range(N+1)) + D*x
print 'u:', simplify(u)
print "u'':", simplify(diff(u, x, x))
print 'BC x=0:', simplify(diff(u, x).subs(x, 0))
print 'BC x=1:', simplify(u.subs(x, 1))
```

The output becomes

```
u: C*x - C + D - x**2 + 1
u'': -2
BC x=0: C
BC x=1: D
```

The complete `sympy` code is found in `u_xx_2_CD.py`[2].

The exact solution is found by integrating twice and applying the boundary conditions, either by hand or using `sympy` as shown in Section 1.2. It appears that the numerical solution coincides with the exact one. This result is to be expected because if $(u_e - B) \in V$, $u = u_e$, as proved next.

2.5 When the numerical method is exact

We have some variational formulation: find $(u - B) \in V$ such that $a(u, v) = L(u)\ \forall V$. The exact solution also fulfills $a(u_e, v) = L(v)$, but normally $(u_e - B)$ lies in a much larger (infinite-dimensional) space. Suppose, nevertheless, that $u_e - B = E$, where $E \in V$. That is, apart from Dirichlet conditions, u_e lies in our finite-dimensional space V we use to compute u. Writing also u on the same form $u = B + F$, $F \in V$, we have

$$\begin{aligned}
a(B + E, v) &= L(v) \quad \forall v \in V,\\
a(B + F, v) &= L(v) \quad \forall v \in V\,.
\end{aligned}$$

[2] http://tinyurl.com/nm5587k/fem/u_xx_2_CD.py

Since these are two variational statements in the same space, we can subtract them and use the bilinear property of $a(\cdot,\cdot)$:

$$a(B+E,v) - a(B+F,v) = L(v) - L(v)$$
$$a(B+E-(B+F),v) = 0$$
$$a(E-F),v) = 0$$

If $a(E-F),v) = 0$ for all v in V, then $E-F$ must be zero everywhere in the domain, i.e., $E=F$. Or in other words: $u = u_{\mathrm{e}}$. This proves that the exact solution is recovered if $u_{\mathrm{e}} - B$ lies in V., i.e., can expressed as $\sum_{j\in\mathcal{I}_s} d_j\psi_j$ if $\{\psi_j\}_{j\in\mathcal{I}_s}$ is a basis for V. The method will then compute the solution $c_j = d_j$, $j\in\mathcal{I}_s$.

The case treated in Section 2.4 is of the type where $u_{\mathrm{e}} - B$ is a quadratic function that is 0 at $x=1$, and therefore $(u_{\mathrm{e}} - B)\in V$, and the method finds the exact solution.

3 Computing with finite elements

The purpose of this section is to demonstrate in detail how the finite element method can the be applied to the model problem

$$-u''(x) = 2, \quad x\in(0,L),\ u(0) = u(L) = 0,$$

with variational formulation

$$(u',v') = (2,v) \quad \forall v\in V\,.$$

The variational formulation is derived in Section 1.10.

3.1 Finite element mesh and basis functions

We introduce a finite element mesh with N_e cells, all with length h, and number the cells from left to right. Choosing P1 elements, there are two nodes per cell, and the coordinates of the nodes become

$$x_i = ih, \quad h = L/N_e, \quad i = 0,\ldots,N_n - 1 = N_e,$$

provided we number the nodes from left to right.

Each of the nodes, i, is associated a finite element basis function $\varphi_i(x)$. When approximating a given function f by a finite element function u, we expand u using finite element basis functions associated with *all* nodes in the mesh. The parameter N, which counts the unknowns from 0 to N then equations $N_n - 1$. However, when solving differential equations we will often have $N < N_n - 1$ because of Dirichlet boundary conditions. Why this is the case will now be explained in detail.

In our case with homogeneous Dirichlet boundary conditions we do not need any boundary function $B(x)$ and can work with the expansion

$$u(x) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\,. \tag{54}$$

Because of the boundary conditions, we must demand $\psi_i(0) = \psi_i(L) = 0$, $i\in\mathcal{I}_s$. When ψ_i for all $i = 0,\ldots,N$ is to be selected among the finite element basis functions φ_j, $i = 0,\ldots,N_n - 1$, we

have to avoid using φ_j functions that do not vanish at $x_0 = 0$ and $x_{N_n-1} = L$. However, all φ_j vanish at these two nodes for $j = 1,\ldots,N_n - 2$. Only basis functions associated with the end nodes, φ_0 and φ_{N_n-1}, violate the boundary conditions of our differential equation. Therefore, we select the basis functions φ_i to be the set of finite element basis functions associated with all the interior nodes in the mesh:

$$\psi_i = \varphi_{i+1}, \quad i = 0,\ldots,N\,.$$

The i index runs over all the unknowns c_i in the expansion for u, and in this case $N = N_n - 3$.

In the general case, the nodes are not necessarily numbered from left to right, so we introduce a mapping from the node numbering, or more precisely the degree of freedom numbering, to the numbering of the unknowns in the final equation system. These unknowns take on the numbers $0,\ldots,N$. Unknown number j in the linear system corresponds to degree of freedom number $\nu(j)$, $j\in\mathcal{I}_s$. We can then write

$$\psi_i = \varphi_{\nu(i)}, \quad i = 0,\ldots,N\,.$$

With a regular numbering as in the present example, $\nu(j) = j+1$, $j = 0,\ldots,N = N_n - 3$.

3.2 Computation in the global physical domain

We shall first perform a computation in the x coordinate system because the integrals can be easily computed here by simple, visual, geometric considerations. This is called a global approach since we work in the x coordinate system and compute integrals on the global domain $[0,L]$.

The entries in the coefficient matrix and right-hand side are

$$A_{i,j} = \int_0^L \psi_i'(x)\psi_j'(x)\,\mathrm{d}x, \quad b_i = \int_0^L 2\psi_i(x)\,\mathrm{d}x, \quad i,j\in\mathcal{I}_s\,.$$

Expressed in terms of finite element basis functions φ_i we get the alternative expressions

$$A_{i,j} = \int_0^L \varphi_{i+1}'(x)\varphi_{j+1}'(x)\,\mathrm{d}x, \quad b_i = \int_0^L 2\varphi_{i+1}(x)\,\mathrm{d}x, \quad i,j\in\mathcal{I}_s\,.$$

For the following calculations the subscripts on the finite element basis functions are more conveniently written as i and j instead of $i+1$ and $j+1$, so our notation becomes

$$A_{i-1,j-1} = \int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x, \quad b_{i-1} = \int_0^L 2\varphi_i(x)\,\mathrm{d}x,$$

where the i and j indices run as $i,j = 1,\ldots,N+1 = N_n - 2$.

The $\varphi_i(x)$ function is a hat function with peak at $x = x_i$ and a linear variation in $[x_{i-1},x_i]$ and $[x_i,x_{i+1}]$. The derivative is $1/h$ to the left of x_i and $-1/h$ to the right, or more formally,

$$\varphi_i'(x) = \begin{cases} 0, & x < x_{i-1},\\ h^{-1}, & x_{i-1}\le x < x_i,\\ -h^{-1}, & x_i\le x < x_{i+1},\\ 0, & x\ge x_{i+1}\end{cases} \tag{55}$$

Figure 2 shows $\varphi_2'(x)$ and $\varphi_3'(x)$.

We realize that φ_i' and φ_j' has no overlap, and hence their product vanishes, unless i and j are nodes belonging to the same cell. The only nonzero contributions to the coefficient matrix are therefore

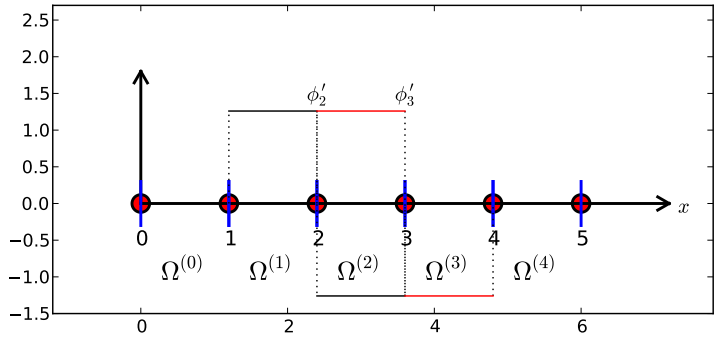


Figure 2: Illustration of the derivative of piecewise linear basis functions associated with nodes in cell 2.

$$
\begin{aligned}
A_{i-1,i-2} &= \int_0^L \varphi_i'(x)\varphi_{i-1}'(x)\,\mathrm{d}x,\\
A_{i-1,i-1} &= \int_0^L \varphi_i'(x)^2\,\mathrm{d}x,\\
A_{i-1,i} &= \int_0^L \varphi_i'(x)\varphi_{i+1}'(x)\,\mathrm{d}x,
\end{aligned}
$$

for $i = 1, \ldots, N+1$, but for $i = 1$, $A_{i-1,i-2}$ is not defined, and for $i = N+1$, $A_{i-1,i}$ is not defined.

We see that $\varphi_{i-1}'(x)$ and $\varphi_i'(x)$ have overlap of one cell $\Omega^{(i-1)} = [x_{i-1}, x_i]$ and that their product then is $-1/h^2$. The integrand is constant and therefore $A_{i-1,i-2} = -h^{-2}h = -h^{-1}$. A similar reasoning can be applied to $A_{i-1,i}$, which also becomes $-h^{-1}$. The integral of $\varphi_i'(x)^2$ gets contributions from two cells, $\Omega^{(i-1)} = [x_{i-1}, x_i]$ and $\Omega^{(i)} = [x_i, x_{i+1}]$, but $\varphi_i'(x)^2 = h^{-2}$ in both cells, and the length of the integration interval is $2h$ so we get $A_{i-1,i-1} = 2h^{-1}$.

The right-hand side involves an integral of $2\varphi_i(x)$, $i = 1, \ldots, N_n - 2$, which is just the area under a hat function of height 1 and width $2h$, i.e., equal to h. Hence, $b_{i-1} = 2h$.

To summarize the linear system, we switch from i to $i+1$ such that we can write

$$
A_{i,i-1} = A_{i,i+1} = -h^{-1}, \quad A_{i,i} = 2h^{-1}, \quad b_i = 2h\,.
$$

The equation system to be solved only involves the unknowns c_i for $i \in \mathcal{I}_s$. With our numbering of unknowns and nodes, we have that c_i equals $u(x_{i+1})$. The complete matrix system that takes the following form:

$$
\frac{1}{h}\begin{pmatrix}
1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0\\
-1 & 2 & -1 & \ddots & & & & & \vdots\\
0 & -1 & 2 & -1 & \ddots & & & & \vdots\\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots\\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots\\
\vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots\\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0\\
\vdots & & & & & \ddots & \ddots & \ddots & -1\\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 1
\end{pmatrix}
\begin{pmatrix} c_0\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ c_N \end{pmatrix}
=
\begin{pmatrix} 2h\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ 2h \end{pmatrix}
\tag{56}
$$

3.3 Comparison with a finite difference discretization

A typical row in the matrix system can be written as

$$
-\frac{1}{h}c_{i-1} + \frac{2}{h}c_i - \frac{1}{h}c_{i+1} = 2h\,. \tag{57}
$$

Let us introduce the notation u_j for the value of u at node j: $u_j = u(x_j)$ since we have the interpretation $u(x_j) = \sum_j c_j\varphi(x_j) = \sum_j c_j\delta_{ij} = c_j$. The unknowns $c_0, \ldots, c_N$ are $u_1, \ldots, u_{N_n-2}$. Shifting i with $i+1$ in (57) and inserting $u_i = c_{i-1}$, we get

$$
-\frac{1}{h}u_{i-1} + \frac{2}{h}u_i - \frac{1}{h}u_{i+1} = 2h, \tag{58}
$$

A finite difference discretization of $-u''(x) = 2$ by a centered, second-order finite difference approximation $u''(x_i) \approx [D_xD_xu]_i$ with $\Delta x = h$ yields

$$
-\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} = 2, \tag{59}
$$

which is, in fact, equivalent to (58) if (58) is divided by h. Therefore, the finite difference and the finite element method are equivalent in this simple test problem.

Sometimes a finite element method generates the finite difference equations on a uniform mesh, and sometimes the finite element method generates equations that are different. The differences are modest, but may influence the numerical quality of the solution significantly, especially in time-dependent problems.

3.4 Cellwise computations

We now employ the cell by cell computational procedure where an element matrix and vector are calculated for each cell and assembled in the global linear system. All integrals are mapped to the local reference coordinate system $X \in [-1, 1]$. In the present case, the matrix entries contain derivatives with respect to x,

$$
A^{(e)}_{i-1,j-1} = \int_{\Omega^{(e)}} \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x = \int_{-1}^{1} \frac{d}{dx}\tilde{\varphi}_r(X)\frac{d}{dx}\tilde{\varphi}_s(X)\frac{h}{2}\,\mathrm{d}X,
$$

where the global degree of freedom i is related to the local degree of freedom r through $i = q(e, r)$. Similarly, $j = q(e, s)$. The local degrees of freedom run as $r, s = 0, 1$ for a P1 element.

The integral for the element matrix. There are simple formulas for the basis functions $\tilde{\varphi}_r(X)$ as functions of X. However, we now need to find the derivative of $\tilde{\varphi}_r(X)$ with respect to x. Given

$$\tilde{\varphi}_0(X) = \frac{1}{2}(1-X), \quad \tilde{\varphi}_1(X) = \frac{1}{2}(1+X),$$

we can easily compute $d\tilde{\varphi}_r/dX$:

$$\frac{d\tilde{\varphi}_0}{dX} = -\frac{1}{2}, \quad \frac{d\tilde{\varphi}_1}{dX} = \frac{1}{2}\,.$$

From the chain rule,

$$\frac{d\tilde{\varphi}_r}{dx} = \frac{d\tilde{\varphi}_r}{dX}\frac{dX}{dx} = \frac{2}{h}\frac{d\tilde{\varphi}_r}{dX}\,. \tag{60}$$

The transformed integral is then

$$A^{(e)}_{i-1,j-1} = \int_{\Omega^{(e)}} \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x = \int_{-1}^{1} \frac{2}{h}\frac{d\tilde{\varphi}_r}{dX}\frac{2}{h}\frac{d\tilde{\varphi}_s}{dX}\frac{h}{2}\,\mathrm{d}X\,.$$

The integral for the element vector. The right-hand side is transformed according to

$$b^{(e)}_{i-1} = \int_{\Omega^{(e)}} 2\varphi_i(x)\,\mathrm{d}x = \int_{-1}^{1} 2\tilde{\varphi}_r(X)\frac{h}{2}\,\mathrm{d}X, \quad i = q(e,r),\ r = 0,1\,.$$

Detailed calculations of the element matrix and vector. Specifically for P1 elements we arrive at the following calculations for the element matrix entries:

$$\begin{aligned}
\tilde{A}^{(e)}_{0,0} &= \int_{-1}^{1} \frac{2}{h}\left(-\frac{1}{2}\right)\frac{2}{h}\left(-\frac{1}{2}\right)\frac{h}{2}\,\mathrm{d}X = \frac{1}{h}\\
\tilde{A}^{(e)}_{0,1} &= \int_{-1}^{1} \frac{2}{h}\left(-\frac{1}{2}\right)\frac{2}{h}\left(\frac{1}{2}\right)\frac{h}{2}\,\mathrm{d}X = -\frac{1}{h}\\
\tilde{A}^{(e)}_{1,0} &= \int_{-1}^{1} \frac{2}{h}\left(\frac{1}{2}\right)\frac{2}{h}\left(-\frac{1}{2}\right)\frac{h}{2}\,\mathrm{d}X = -\frac{1}{h}\\
\tilde{A}^{(e)}_{1,1} &= \int_{-1}^{1} \frac{2}{h}\left(\frac{1}{2}\right)\frac{2}{h}\left(\frac{1}{2}\right)\frac{h}{2}\,\mathrm{d}X = \frac{1}{h}
\end{aligned}$$

The element vector entries become

$$\begin{aligned}
\tilde{b}^{(e)}_0 &= \int_{-1}^{1} 2\frac{1}{2}(1-X)\frac{h}{2}\,\mathrm{d}X = h\\
\tilde{b}^{(e)}_1 &= \int_{-1}^{1} 2\frac{1}{2}(1+X)\frac{h}{2}\,\mathrm{d}X = h\,.
\end{aligned}$$

Expressing these entries in matrix and vector notation, we have

$$\tilde{A}^{(e)} = \frac{1}{h}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \tilde{b}^{(e)} = h\begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{61}$$

Contributions from the first and last cell. The first and last cell involve only one unknown and one basis function because of the Dirichlet boundary conditions at the first and last node. The element matrix therefore becomes a 1×1 matrix and there is only one entry in the element vector. On cell 0, only $\psi_0 = \varphi_1$ is involved, corresponding to integration with $\tilde{\varphi}_1$. On cell N_e, only $\psi_N = \varphi_{N_n-2}$ is involved, corresponding to integration with $\tilde{\varphi}_0$. We then get the special end-cell contributions

$$\tilde{A}^{(e)} = \frac{1}{h}\begin{pmatrix} 1 \end{pmatrix}, \quad \tilde{b}^{(e)} = h\begin{pmatrix} 1 \end{pmatrix}, \tag{62}$$

for $e = 0$ and $e = N_e$. In these cells, we have only one degree of freedom, not two as in the interior cells.

Assembly. The next step is to assemble the contributions from the various cells. The assembly of an element matrix and vector into the global matrix and right-hand side can be expressed as

$$A_{q(e,r),q(e,s)} = A_{q(e,r),q(e,s)} + \tilde{A}^{(e)}_{r,s}, \quad b_{q(e,r)} = b_{q(e,r)} + \tilde{b}^{(e)}_r,$$

for r and s running over all local degrees of freedom in cell e.

To make the assembly algorithm more precise, it is convenient to set up Python data structures and a code snippet for carrying out all details of the algorithm. For a mesh of four equal-sized P1 elements and $L = 2$ we have

```
vertices = [0, 0.5, 1, 1.5, 2]
cells = [[0, 1], [1, 2], [2, 3], [3, 4]]
dof_map = [[0], [0, 1], [1, 2], [2]]
```

The total number of degrees of freedom is 3, being the function values at the internal 3 nodes where u is unknown. In cell 0 we have global degree of freedom 0, the next cell has u unknown at its two nodes, which become global degrees of freedom 0 and 1, and so forth according to the `dof_map` list. The mathematical $q(e,r)$ quantity is nothing but the `dof_map` list.

Assume all element matrices are stored in a list `Ae` such that `Ae[e][i,j]` is $\tilde{A}^{(e)}_{i,j}$. A corresponding list for the element vectors is named `be`, where `be[e][r]` is $\tilde{b}^{(e)}_r$. A Python code snippet illustrates all details of the assembly algorithm:

```
# A[i,j]: coefficient matrix, b[i]: right-hand side
for e in range(len(Ae)):
    for r in range(Ae[e].shape[0]):
        for s in range(Ae[e].shape[1]):
            A[dof_map[e,r],dof_map[e,s]] += Ae[e][i,j]
        b[dof_map[e,r]] += be[e][i,j]
```

The general case with `N_e` P1 elements of length `h` has

```
N_n = N_e + 1
vertices = [i*h for i in range(N_n)]
cells = [[e, e+1] for e in range(N_e)]
dof_map = [[0]] + [[e-1, e] for i in range(1, N_e)] + [[N_n-2]]
```

Carrying out the assembly results in a linear system that is identical to (56), which is not surprising since the procedures is mathematically equivalent to the calculations in the physical domain.

A fundamental problem with the matrix system we have assembled is that the boundary conditions are not incorporated if $u(0)$ or $u(L)$ are different from zero. The next sections deals with this issue.

4 Boundary conditions: specified nonzero value

We have to take special actions to incorporate Dirichlet conditions, such as $u(L) = D$, into the computational procedures. The present section outlines alternative, yet mathematically equivalent, methods.

4.1 General construction of a boundary function

In Section 1.11 we introduce a boundary function $B(x)$ to deal with nonzero Dirichlet boundary conditions for u. The construction of such a function is not always trivial, especially not in multiple dimensions. However, a simple and general construction idea exists when the basis functions have the property

$$\varphi_i(x_j) = \delta_{ij}, \quad \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

where x_j is a boundary point. Examples on such functions are the Lagrange interpolating polynomials and finite element functions.

Suppose now that u has Dirichlet boundary conditions at nodes with numbers $i \in I_b$. For example, $I_b = \{0, N_n - 1\}$ in a 1D mesh with node numbering from left to right and Dirichlet conditions at the end nodes $i = 0$ and $i = N_n - 1$. Let U_i be the corresponding prescribed values of $u(x_i)$. We can then, in general, use

$$B(x) = \sum_{j \in I_b} U_j \varphi_j(x)\,. \tag{63}$$

It is easy to verify that $B(x_i) = \sum_{j \in I_b} U_j \varphi_j(x_i) = U_i$.

The unknown function can then be written as

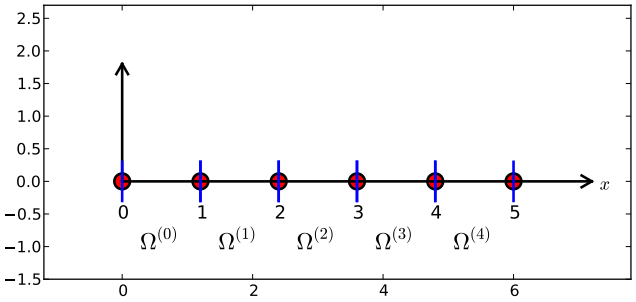
$$u(x) = \sum_{j \in I_b} U_j \varphi_j(x) + \sum_{j \in \mathcal{I}_s} c_j \varphi_{\nu(j)}, \tag{64}$$

where $\nu(j)$ maps unknown number j in the equation system to node $\nu(j)$. We can easily show that with this u, a Dirichlet condition $u(x_k) = U_k$ is fulfilled:

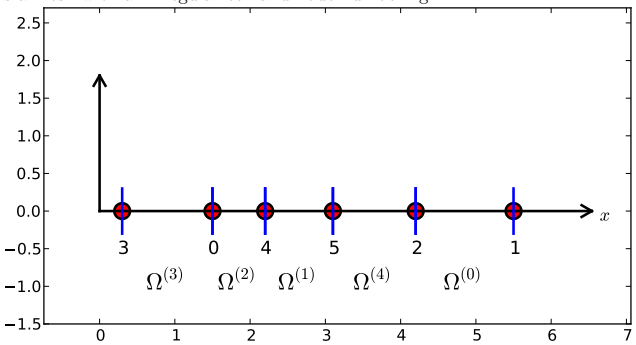
$$u(x_k) = \sum_{j \in I_b} U_j \underbrace{\varphi_j(x)}_{\neq 0 \text{ only for } j=k} + \sum_{j \in \mathcal{I}_s} c_j \underbrace{\varphi_{\nu(j)}(x_k)}_{=0,\ k \notin \mathcal{I}_s} = U_k$$

Some examples will further clarify the notation. With a regular left-to-right numbering of nodes in a mesh with P1 elements, and Dirichlet conditions at $x = 0$, we use finite element basis functions associated with the nodes $1, 2, \ldots, N_n - 1$, implying that $\nu(j) = j + 1$, $j = 0, \ldots, N$, where $N = N_n - 2$. For the particular mesh below the expansion becomes

$$u(x) = U_0\varphi_0(x) + c_0\varphi_1(x) + c_1\varphi_2(x) + \cdots + c_4\varphi_5(x)\,.$$



Here is a mesh with an irregular cell and node numbering:



Say we in this latter mesh have Dirichlet conditions on the left-most and right-most node, with numbers 3 and 1, respectively. Then we can number the unknowns at the interior nodes from left to right, giving $\nu(0) = 0$, $\nu(1) = 4$, $\nu(2) = 5$, $\nu(3) = 2$. This gives

$$B(x) = U_3\varphi_3(x) + U_1\varphi_1(x),$$

and

$$u(x) = B(x) + \sum_{j=0}^{3} c_j\varphi_{\nu(j)} = U_3\varphi_3 + U_1\varphi_1 + c_0\varphi_0 + c_1\varphi_4 + c_2\varphi_5 + c_3\varphi_2\,.$$

Switching to the more standard case of left-to-right numbering and boundary conditions $u(0) = C$, $u(L) = D$, we have $N = N_n - 3$ and

$$\begin{aligned} u(x) &= C\varphi_0 + D\varphi_{N_n-1} + \sum_{j \in \mathcal{I}_s} c_j\varphi_{j+1} \\ &= C\varphi_0 + D\varphi_{N_n} + c_0\varphi_1 + c_1\varphi_2 + \cdots + c_N\varphi_{N_n-2}\,. \end{aligned}$$

The idea of constructing B described here generalizes almost trivially to 2D and 3D problems: $B = \sum_{j \in I_b} U_j\varphi_j$, where I_b is the index set containing the numbers of all the nodes on the boundaries where Dirichlet values are prescribed.

4.2 Example on computing with finite element-based a boundary function

Let us see how the model problem $-u'' = 2$, $u(0) = C$, $u(L) = D$, is affected by a $B(x)$ to incorporate boundary values. Inserting the expression

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)$$

in $-(u'', \psi_i) = (f, \psi_i)$ and integrating by parts results in a linear system with

$$A_{i,j} = \int_0^L \psi_i'(x)\psi_j'(x)\,\mathrm{d}x, \quad b_i = \int_0^L (f(x)\psi_i(x) - B'(x)\psi_i'(x))\,\mathrm{d}x\,.$$

We choose $\psi_i = \varphi_{i+1}$, $i = 0, \ldots, N = N_n - 3$ if the node numbering is from left to right. (Later we also need the assumption that the cells too are numbered from left to right.) The boundary function becomes

$$B(x) = C\varphi_0(x) + D\varphi_{N_n-1}(x)\,.$$

The expansion for $u(x)$ is

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\varphi_{j+1}(x)\,.$$

We can write the matrix and right-hand side entries as

$$A_{i-1,j-1} = \int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x, \quad b_{i-1} = \int_0^L (f(x) - C\varphi_0'(x) - D\varphi_{N_n-1}'(x))\varphi_i'(x)\,\mathrm{d}x,$$

for $i, j = 1, \ldots, N + 1 = N_n - 2$. Note that we have here used $B' = C\varphi_0' + D\varphi_{N_n-1}'$.

Computations in physical coordinates. Most of the terms in the linear system have already been computed so we concentrate on the new contribution from the boundary function. The integral $C\int_0^L \varphi_0'(x))\varphi_i'(x)\,\mathrm{d}x$ can only get a nonzero contribution from the first cell, $\Omega^{(0)} = [x_0, x_1]$ since $\varphi_0'(x) = 0$ on all other cells. Moreover, $\varphi_0'(x)\varphi_i'(x)\,\mathrm{d}x \neq 0$ only for $i = 0$ and $i = 1$ (but $i = 0$ is excluded), since $\varphi_i = 0$ on the first cell if $i > 1$. With a similar reasoning we realize that $D\int_0^L \varphi_{N_n-1}'(x))\varphi_i'(x)\,\mathrm{d}x$ can only get a nonzero contribution from the last cell. From the explanations of the calculations in Section **??** in [1] we then find that

$$\int_0^L \varphi_0'(x)\varphi_1'(x)\,\mathrm{d}x = (-\frac{1}{h})\cdot\frac{1}{h}\cdot h = -\frac{1}{h}, \quad \int_0^L \varphi_{N_n-1}'(x)\varphi_{N_n-2}'(x)\,\mathrm{d}x = \frac{1}{h}\cdot(-\frac{1}{h})\cdot h = -\frac{1}{2}\,.$$

The extra boundary term because of $B(x)$ boils down to adding C/h to b_0 and D/h to b_N.

Cellwise computations on the reference element. As an equivalent alternative, we now turn to cellwise computations. The element matrices and vectors are calculated as Section 3.4, so we concentrate on the impact of the new term involving $B(x)$. We observe that $C\varphi_0' = 0$ on all cells except $e = 0$, and $D\varphi_{N_n-1}' = 0$ on all cells except $e = N_e$. In this case there is only one unknown in these cells since $u(0)$ and $u(L)$ are prescribed, so the element vector has only one entry. The entry for the last cell, $e = N_e$, becomes

$$\tilde{b}_0^{(e)} = \int_{-1}^1 \left(f - D\frac{2}{h}\frac{d\tilde{\varphi}_1}{dX}\right)\tilde{\varphi}_0\frac{h}{2}\,\mathrm{d}X = (\frac{h}{2}(2 - D\frac{2}{h}\frac{1}{2})\int_{-1}^1 \tilde{\varphi}_0\,\mathrm{d}X = h - D/2\,.$$

Similar computations on the first cell yield

$$\tilde{b}_0^{(0)} = \int_{-1}^1 \left(f - C\frac{2}{h}\frac{d\tilde{\varphi}_0}{dX}\right)\tilde{\varphi}_1\frac{h}{2}\,\mathrm{d}X = (\frac{h}{2}(2 + C\frac{2}{h}\frac{1}{2})\int_{-1}^1 \tilde{\varphi}_1\,\mathrm{d}X = h + C/2\,.$$

When assembling these contributions, we see that b_0 gets right-hand side of the linear system gets an extra term $C/2$ and b_N gets $-D/2$, as in the computations in the physical domain.

4.3 Modification of the linear system

From an implementational point of view, there is a convenient alternative to adding the $B(x)$ function and using only the basis functions associated with nodes where u is truly unknown. Instead of seeking

$$u(x) = \sum_{j\in I_b} U_j\varphi_j(x) + \sum_{j\in\mathcal{I}_s} c_j\varphi_{\nu(j)}(x), \tag{65}$$

we use the sum over all degrees of freedom, including the known boundary values:

$$u(x) = \sum_{j\in\mathcal{I}_s} c_j\varphi_j(x)\,. \tag{66}$$

Note that the collections of unknowns $\{c_i\}_{i\in\mathcal{I}_s}$ in (65) and (66) are different: in (65) the unknowns correspond to nodes where u is not known, while in (65) the unknowns cover u values at all the nodes.

The idea is to compute the entries in the linear system as if no Dirichlet values are prescribed. Afterwards, we modify the linear system to ensure that the known c_j values are incorporated.

A potential problem arises for the boundary term $[u'v]_0^L$ from the integration by parts: imagining no Dirichlet conditions means that we no longer require $v = 0$ at Dirichlet points, and the boundary term is then nonzero at these points. However, when we modify the linear system, we will erase whatever the contribution from $[u'v]_0^L$ should be at the Dirichlet points in the right-hand side of the linear system. We can therefore safely forget $[u'v]_0^L$ at any point where a Dirichlet condition applies.

Computations in the physical system. Let us redo the computations in the example in Section 4.1. We solve $-u'' = 2$ with $u(0) = 0$ and $u(L) = D$. The expressions for $A_{i,j}$ and b_i are the same, but the numbering is different as the numbering of unknowns and nodes now coincide:

$$A_{i,j} = \int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x, \quad b_i = \int_0^L f(x)\varphi_i(x)\,\mathrm{d}x,$$

for $i, j = 0, \ldots, N = N_n - 1$. The integrals involving basis functions corresponding to interior mesh nodes, $i, j = 1, \ldots, N_n - 2$, are obviously the same as before. We concentrate on the contributions from φ_0 and φ_{N_n-1}:

$$A_{0,0} = \int_0^L (\varphi_0')^2 \,\mathrm{d}x = \int_0^{x_1} = (\varphi_0')^2 \,\mathrm{d}x \frac{1}{h},$$
$$A_{0,1} = \int_0^L \varphi_0'\varphi_1' \,\mathrm{d}x = \int_0^{x_1} \varphi_0'\varphi_1' \,\mathrm{d}x = -\frac{1}{h},$$
$$A_{N,N} = \int_0^L (\varphi_N')^2 \,\mathrm{d}x = \int_{x_{N_n-2}}^{x_{N_n-1}} (\varphi_N')^2 \,\mathrm{d}x = \frac{1}{h},$$
$$A_{N,N-1} = \int_0^L \varphi_N'\varphi_{N-1}' \,\mathrm{d}x = \int_{x_{N_n-2}}^{x_{N_n-1}} \varphi_N'\varphi_{N-1}' \,\mathrm{d}x = -\frac{1}{h}\,.$$

The new terms on the right-hand side are also those involving φ_0 and φ_{N_n-1}:

$$b_0 = \int_0^L 2\varphi_0(x) \,\mathrm{d}x = \int_0^{x_1} 2\varphi_0(x) \,\mathrm{d}x = h,$$
$$b_N = \int_0^L 2\varphi_{N_n-1} \,\mathrm{d}x = \int_{x_{N_n-2}}^{x_{N_n-1}} 2\varphi_{N_n-1} \,\mathrm{d}x = h\,.$$

The complete matrix system, involving all degrees of freedom, takes the form

$$\frac{1}{h}\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & & & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} h \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h \\ h \end{pmatrix} \tag{67}$$

Incorporation of Dirichlet values can now be done by replacing the first and last equation by $c_0 = 0$ and $c_N = D$. This action changes the system to

$$\frac{1}{h}\begin{pmatrix} h & 0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & & & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & h \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} 0 \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h \\ D \end{pmatrix} \tag{68}$$

Note that because we do not require $\varphi_i(0) = 0$ and $\varphi_i(L)$, $i \in \mathcal{I}_s$, the boundary term $[u'v]_0^L$ gives in principle contributions $u'(0)\varphi_0(0)$ to b_0 and $u'(L)\varphi_N(L)$ to b_N ($u'\varphi_i$ vanishes for $x = 0$ or $x = L$ for $i = 1, \ldots, N-1$). Nevertheless, we erase these contributions in b_0 and b_N and insert boundary values instead. This argument shows why we can drop computing $[u'v]_0^L$ at Dirichlet nodes when we implement the Dirichlet values by modifying the linear system.

4.4 Symmetric modification of the linear system

The original matrix system (56) is symmetric, but the modifications in (68) destroy the symmetry. Our described modification will in general destroy an initial symmetry in the matrix system. This is not a particular computational disadvantage for tridiagonal systems arising in 1D problems, but may be more serious in 2D and 3D problems when the systems are large and exploiting symmetry can be important for halving the storage demands, speeding up computations, and/or making the solution algorithm more robust. Therefore, an alternative modification which preserves symmetry is frequently applied.

Let c_k be a coefficient corresponding to a known value $u(x_k) = U_k$. We want to replace equation k in the system by $c_k = U_k$, i.e., insert zeroes in row number k in the coefficient matrix, set 1 on the diagonal, and replace b_k by U_k. A symmetry-preserving modification consists in first subtracting column number k in the coefficient matrix, i.e., $A_{i,k}$ for $i \in \mathcal{I}_s$, times the boundary value U_k, from the right-hand side: $b_i \leftarrow b_i - A_{i,k}U_k$. Then we put zeroes in row number k *and* column number k in the coefficient matrix, and finally set $b_k = U_k$. The steps in algorithmic form becomes

1. $b_i \leftarrow b_i - A_{i,k}U_k$ for $i \in \mathcal{I}_s$
2. $A_{i,k} = A_{k,i} = 0$ for $i \in \mathcal{I}_s$
3. $A_{k,k} = 1$
4. $b_i = U_k$

This modification goes as follows for the specific linear system written out in (67) in Section 4.3. First we subtract the first column in the coefficient matrix, times the boundary value, from the right-hand side. Because $c_0 = 0$, this subtraction has no effect. Then we subtract the last column, times the boundary value D, from the right-hand side. This action results in $b_{N-1} = 2h + D/h$ and $b_N = h - 2D/h$. Thereafter, we place zeros in the first and last row and column in the coefficient matrix and 1 on the two corresponding diagonal entries. Finally, we set $b_0 = 0$ and $b_N = D$. The result becomes

$$\frac{1}{h}\begin{pmatrix} h & 0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 2 & -1 & \ddots & & & & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & h \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} 0 \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h + D/h \\ D \end{pmatrix} \tag{69}$$

4.5 Modification of the element matrix and vector

The modifications of the global linear system can alternatively be done for the element matrix and vector. (The assembled system will get the value n on the main diagonal if n elements contribute to the same unknown, but the factor n will also appear on the right-hand side and hence cancel out.)

We have, in the present computational example, the element matrix and vector (61). The modifications are needed in cells where one of the degrees of freedom is known. Here, this means the first and last cell. We compute the element matrix and vector as there are no Dirichlet conditions. The boundary term $[u'v]_0^L$ is simply forgotten at nodes that have Dirichlet conditions because the modification of the element vector will anyway erase the contribution from the boundary term. In the first cell, local degree of freedom number 0 is known and the modification becomes

$$\tilde{A}^{(0)} = A = \frac{1}{h}\begin{pmatrix} h & 0 \\ -1 & 1 \end{pmatrix}, \quad \tilde{b}^{(0)} = \begin{pmatrix} 0 \\ h \end{pmatrix}. \tag{70}$$

In the last cell we set

$$\tilde{A}^{(N_e)} = A = \frac{1}{h}\begin{pmatrix} 1 & -1 \\ 0 & h \end{pmatrix}, \quad \tilde{b}^{(N_e)} = \begin{pmatrix} h \\ D \end{pmatrix}. \tag{71}$$

We can also perform the symmetric modification. This operation affects only the last cell with a nonzero Dirichlet condition. The algorithm is the same as for the global linear system, resulting in

$$\tilde{A}^{(N_e)} = A = \frac{1}{h}\begin{pmatrix} 1 & 0 \\ 0 & h \end{pmatrix}, \quad \tilde{b}^{(N_e)} = \begin{pmatrix} h + D/h \\ D \end{pmatrix}. \tag{72}$$

The reader is encouraged to assemble the element matrices and vectors and check that the result coincides with the system (69).

5 Boundary conditions: specified derivative

Suppose our model problem $-u''(x) = f(x)$ features the boundary conditions $u'(0) = C$ and $u(L) = D$. As already indicated in Section 2, the former condition can be incorporated through the boundary term that arises from integration by parts. This details of this method will now be illustrated in the context of finite element basis functions.

5.1 The variational formulation

Starting with the Galerkin method,

$$\int_0^L (u''(x) + f(x))\psi_i(x)\,\mathrm{d}x = 0, \quad i \in \mathcal{I}_s,$$

integrating $u''\psi_i$ by parts results in

$$\int_0^L u'(x)'\psi_i'(x)\,\mathrm{d}x - (u'(L)\psi_i(L) - u'(0)\psi_i(0)) = \int_0^L f(x)\psi_i(x)\,\mathrm{d}x, \quad i \in \mathcal{I}_s\,.$$

The first boundary term, $u'(L)\psi_i(L)$, vanishes because $u(L) = D$. There are two arguments for this result, explained in detail below. The second boundary term, $u'(0)\psi_i(0)$, can be used to

implement the condition $u'(0) = C$, provided $\psi_i(0) \neq 0$ for some i (but with finite elements we fortunately have $\psi_0(0) = 1$). The variational form of the differential equation then becomes

$$\int_0^L u'(x)\varphi_i'(x)\,\mathrm{d}x + C\varphi_i(0) = \int_0^L f(x)\varphi_i(x)\,\mathrm{d}x, \quad i \in \mathcal{I}_s\,.$$

5.2 Boundary term vanishes because of the test functions

At points where u is known we may require ψ_i to vanish. Here, $u(L) = D$ and then $\psi_i(L) = 0$, $i \in \mathcal{I}_s$. Obviously, the boundary term $u'(L)\psi_i(L)$ then vanishes.

The set of basis functions $\{\psi_i\}_{i\in\mathcal{I}_s}$ contains in this case all the finite element basis functions on the mesh, expect the one that is 1 at $x = L$. The basis function that is left out is used in a boundary function $B(x)$ instead. With a left-to-right numbering, $\psi_i = \varphi_i$, $i = 0, \ldots, N_n - 2$, and $B(x) = D\varphi_{N_n-1}$:

$$u(x) = D\varphi_{N_n-1}(x) + \sum_{j=0}^{N=N_n-2} c_j\varphi_j(x)\,.$$

Inserting this expansion for u in the variational form (5.1) leads to the linear system

$$\sum_{j=0}^{N}\left(\int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x\right)c_j = \int_0^L \left(f(x)\varphi_i(x) - D\varphi_{N_n-1}'(x)\varphi_i'(x)\right)\,\mathrm{d}x - C\varphi_i(0), \tag{73}$$

for $i = 0, \ldots, N = N_n - 2$.

5.3 Boundary term vanishes because of linear system modifications

We may, as an alternative to the approach in the previous section, use a basis $\{\psi_i\}_{i\in\mathcal{I}_s}$ which contains all the finite element functions on the mesh: $\psi_i = \varphi_i$, $i = 0, \ldots, N_n - 1 = N$. In this case, $u'(L)\psi_i(L) = u'(L)\varphi_i(L) \neq 0$ for the i corresponding to the boundary node at $x = L$ (where $\varphi_i = 1$). The number of this node is $i = N_n - 1 = N$ if a left-to-right numbering of nodes is utilized.

However, even though $u'(L)\varphi_{N_n-1}(L) \neq 0$, we do not need to compute this term. For $i < N_n - 1$ we realize that $\varphi_i(L) = 0$. The only nonzero contribution to the right-hand side from the affects b_{N_n-1} ($i = N$). Without a boundary function we must implement the condition $u(L) = D$ by the equivalent statement $c_N = D$ and modify the linear system accordingly. This modification will erase the last row and replace b_N by another value. Any attempt to compute the boundary term $u'(L)\varphi_{N_n-1}(L)$ and store it in b_N will be lost. Therefore, we can safely forget about boundary terms corresponding to Dirichlet boundary conditions also when we use the methods from Section 4.3 or Section 4.4.

The expansion for u reads

$$u(x) = \sum_{j\in\mathcal{I}_s} c_j\varphi_j(x)\,.$$

Insertion in the variational form (5.1) leads to the linear system

$$\sum_{j\in\mathcal{I}_s}\left(\int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x\right)c_j = \int_0^L \left(f(x)\varphi_i(x)\right)\,\mathrm{d}x - C\varphi_i(0), \quad i \in \mathcal{I}_s\,. \tag{74}$$

After having computed the system, we replace the last row by $c_N = D$, either straightforwardly as in Section 4.3 or in a symmetric fashion as in Section 4.4. These modifications can also be performed in the element matrix and vector for the right-most cell.

5.4 Direct computation of the global linear system

We now turn to actual computations with P1 finite elements. The focus is on how the linear system and the element matrices and vectors are modified by the condition $u'(0) = C$.

Consider first the approach where Dirichlet conditions are incorporated by a $B(x)$ function and the known degree of freedom C_{N_n-1} is left out from the linear system (see Section 5.2). The relevant formula for the linear system is given by (73). There are three differences compared to the extensively computed case where $u(0) = 0$ in Sections 3.2 and 3.4. First, because we do not have a Dirichlet condition at the left boundary, we need to extend the linear system (56) with an equation associated with the node $x_0 = 0$. According to Section 4.3, this extension consists of including $A_{0,0} = 1/h$, $A_{0,1} = -1/h$, and $b_0 = h$. For $i > 0$ we have $A_{i,i} = 2/h$, $A_{i-1,i} = A_{i,i+1} = -1/h$. Second, we need to include the extra term $-C\varphi_i(0)$ on the right-hand side. Since all $\varphi_i(0) = 0$ for $i = 1, \ldots, N$, this term reduces to $-C\varphi_0(0) = -C$ and affects only the first equation ($i = 0$). We simply add $-C$ to b_0 such that $b_0 = h - C$. Third, the boundary term $-\int_0^L D\varphi_{N_n-1}(x)\varphi_i \,\mathrm{d}x$ must be computed. Since $i = 0, \ldots, N = N_n - 2$, this integral can only get a nonzero contribution with $i = N_n - 2$ over the last cell. The result becomes $-Dh/6$. The resulting linear system can be summarized in the form

$$\frac{1}{h}\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & & & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} h - C \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h - Dh/6 \end{pmatrix}. \tag{75}$$

Next we consider the technique where we modify the linear system to incorporate Dirichlet conditions (see Section 5.3). Now $N = N_n - 1$. The two differences from the case above is that the $-\int_0^L D\varphi_{N_n-1}\varphi_i \,\mathrm{d}x$ term is left out of the right-hand side and an extra last row associated with the node $x_{N_n-1} = L$ where the Dirichlet condition applies is appended to the system. This last row is anyway replaced by the condition $c_N = D$ or this condition can be incorporated in a symmetric fashion. Using the simplest, former approach gives

$$\frac{1}{h}\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & & & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & h \end{pmatrix}\begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} h - C \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h \\ D \end{pmatrix}. \tag{76}$$

5.5 Cellwise computations

Now we compute with one element at a time, working in the reference coordinate system $X \in [-1, 1]$. We need to see how the $u'(0) = C$ condition affects the element matrix and vector. The extra term $-C\varphi_i(0)$ in the variational formulation only affects the element vector in the first cell. On the reference cell, $-C\varphi_i(0)$ is transformed to $-C\tilde{\varphi}_r(-1)$, where r counts local degrees of freedom. We have $\tilde{\varphi}_0(-1) = 1$ and $\tilde{\varphi}_1(-1) = 0$ so we are left with the contribution $-C\tilde{\varphi}_0(-1) = -C$ to $\tilde{b}_0^{(0)}$:

$$\tilde{A}^{(0)} = A = \frac{1}{h}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \tilde{b}^{(0)} = \begin{pmatrix} h - C \\ h \end{pmatrix}. \tag{77}$$

No other element matrices or vectors are affected by the $-C\varphi_i(0)$ boundary term.

There are two alternative ways of incorporating the Dirichlet condition. Following Section 5.2, we get a 1×1 element matrix in the last cell and an element vector with an extra term containing D:

$$\tilde{A}^{(e)} = \frac{1}{h}\begin{pmatrix} 1 \end{pmatrix}, \quad \tilde{b}^{(e)} = h\begin{pmatrix} 1 - D/6 \end{pmatrix}, \tag{78}$$

Alternatively, we include the degree of freedom at the node with u specified. The element matrix and vector must then be modified to constrain the $\tilde{c}_1 = c_N$ value at local node $r = 1$:

$$\tilde{A}^{(N_e)} = A = \frac{1}{h}\begin{pmatrix} 1 & 1 \\ 0 & h \end{pmatrix}, \quad \tilde{b}^{(N_e)} = \begin{pmatrix} h \\ D \end{pmatrix}. \tag{79}$$

6 Implementation

It is tempting to create a program with symbolic calculations to perform all the steps in the computational machinery, both for automating the work and for documenting the complete algorithms. As we have seen, there are quite many details involved with finite element computations and incorporation of boundary conditions. An implementation will also act as a structured summary of all these details.

6.1 Global basis functions

We first consider implementations when ψ_i are global functions are hence different from zero on most of $\Omega = [0, L]$ so all integrals need integration over the entire domain. Since the expressions for the entries in the linear system depend on the differential equation problem being solved, the user must supply the necessary formulas via Python functions. The implementations here attempt to perform symbolic calculations, but fall back on numerical computations if the symbolic ones fail.

The user must prepare a function `integrand_lhs(psi, i, j)` for returning the integrand of the integral that contributes to matrix entry (i, j). The `psi` variable is a Python dictionary holding the basis functions and their derivatives in symbolic form. More precisely, `psi[q]` is a list of

$$\{\frac{d^q\psi_0}{dx^q}, \ldots, \frac{d^q\psi_{N_n-1}}{dx^q}\}.$$

Similarly, `integrand_rhs(psi, i)` returns the integrand for entry number i in the right-hand side vector.

Since we also have contributions to the right-hand side vector, and potentially also the matrix, from boundary terms without any integral, we introduce two additional functions, `boundary_lhs(psi, i, j)` and `boundary_rhs(psi, i)` for returning terms in the variational formulation that are not to be integrated over the domain Ω. Examples shown later will explain in more detail how these user-supplied function may look like.

The linear system can be computed and solved symbolically by the following function:

```
import sympy as sp

def solve(integrand_lhs, integrand_rhs, psi, Omega,
          boundary_lhs=None, boundary_rhs=None):
    N = len(psi[0]) - 1
    A = sp.zeros((N+1, N+1))
    b = sp.zeros((N+1, 1))
    x = sp.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            integrand = integrand_lhs(psi, i, j)
            I = sp.integrate(integrand, (x, Omega[0], Omega[1]))
            if boundary_lhs is not None:
                I += boundary_lhs(psi, i, j)
            A[i,j] = A[j,i] = I   # assume symmetry
        integrand = integrand_rhs(psi, i)
        I = sp.integrate(integrand, (x, Omega[0], Omega[1]))
        if boundary_rhs is not None:
            I += boundary_rhs(psi, i)
        b[i,0] = I
    c = A.LUsolve(b)
    u = sum(c[i,0]*psi[0][i] for i in range(len(psi[0])))
    return u
```

Not surprisingly, symbolic solution of differential equations, discretized by a Galerkin or least squares method with global basis functions, is of limited interest beyond the simplest problems, because symbolic integration might be very time consuming or impossible, not only in `sympy` but also in WolframAlpha[3] (which applies the perhaps most powerful symbolic integration software available today: Mathematica). Numerical integration as an option is therefore desirable.

[3] `http://wolframalpha.com`

The extended `solve` function below tries to combine symbolic and numerical integration. The latter can be enforced by the user, or it can be invoked after a non-successful symbolic integration (being detected by an `Integral` object as the result of the integration in `sympy`). Note that for a numerical integration, symbolic expressions must be converted to Python functions (using `lambdify`), and the expressions cannot contain other symbols than `x`. The real `solve` routine in the `varform1D.py`[4] file has error checking and meaningful error messages in such cases. The `solve` code below is a condensed version of the real one, with the purpose of showing how to automate the Galerkin or least squares method for solving differential equations in 1D with global basis functions:

```
def solve(integrand_lhs, integrand_rhs, psi, Omega,
          boundary_lhs=None, boundary_rhs=None, symbolic=True):
    N = len(psi[0]) - 1
    A = sp.zeros((N+1, N+1))
    b = sp.zeros((N+1, 1))
    x = sp.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            integrand = integrand_lhs(psi, i, j)
            if symbolic:
                I = sp.integrate(integrand, (x, Omega[0], Omega[1]))
                if isinstance(I, sp.Integral):
                    symbolic = False  # force num.int. hereafter
            if not symbolic:
                integrand = sp.lambdify([x], integrand)
                I = sp.mpmath.quad(integrand, [Omega[0], Omega[1]])
            if boundary_lhs is not None:
                I += boundary_lhs(psi, i, j)
            A[i,j] = A[j,i] = I
        integrand = integrand_rhs(psi, i)
        if symbolic:
            I = sp.integrate(integrand, (x, Omega[0], Omega[1]))
            if isinstance(I, sp.Integral):
                symbolic = False
        if not symbolic:
            integrand = sp.lambdify([x], integrand)
            I = sp.mpmath.quad(integrand, [Omega[0], Omega[1]])
        if boundary_rhs is not None:
            I += boundary_rhs(psi, i)
        b[i,0] = I
    c = A.LUsolve(b)
    u = sum(c[i,0]*psi[0][i] for i in range(len(psi[0])))
    return u
```

6.2 Example: constant right-hand side

To demonstrate the code above, we address

$$-u''(x) = b, \quad x \in \Omega = [0, 1], \quad u(0) = 1,\ u(1) = 0,$$

with b as a (symbolic) constant. A possible basis for the space V is $\psi_i(x) = x^{i+1}(1-x)$, $i \in \mathcal{I}_s$. Note that $\psi_i(0) = \psi_i(1) = 0$ as required by the Dirichlet conditions. We need a $B(x)$ function to take care of the known boundary values of u. Any function $B(x) = 1 - x^p$, $p \in \mathbb{R}$, is a candidate, and one arbitrary choice from this family is $B(x) = 1 - x^3$. The unknown function is then written as

[4] `http://tinyurl.com/nm5587k/fem/varform1D.py`

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\,.$$

Let us use the Galerkin method to derive the variational formulation. Multiplying the differential equation by v and integrate by parts yield

$$\int_0^1 u'v'\,\mathrm{d}x = \int_0^1 fv\,\mathrm{d}x \quad \forall v \in V,$$

and with $u = B + \sum_j c_j\psi_j$ we get the linear system

$$\sum_{j\in\mathcal{I}_s}\left(\int_0^1 \psi_i'\psi_j'\,\mathrm{d}x\right)c_j = \int_0^1 (f\psi_i - B'\psi_i')\,\mathrm{d}x, \quad i\in\mathcal{I}_s\,. \tag{80}$$

The application can be coded as follows in `sympy`:

```
x, b = sp.symbols('x b')
f = b
B = 1 - x**3
dBdx = sp.diff(B, x)

# Compute basis functions and their derivatives
N = 3
psi = {0: [x**(i+1)*(1-x) for i in range(N+1)]}
psi[1] = [sp.diff(psi_i, x) for psi_i in psi[0]]

def integrand_lhs(psi, i, j):
    return psi[1][i]*psi[1][j]

def integrand_rhs(psi, i):
    return f*psi[0][i] - dBdx*psi[1][i]

Omega = [0, 1]

u_bar = solve(integrand_lhs, integrand_rhs, psi, Omega,
              verbose=True, symbolic=True)
u = B + u_bar
print 'solution u:', sp.simplify(sp.expand(u))
```

The printout of `u` reads `-b*x**2/2 + b*x/2 - x + 1`. Note that expanding `u` and then simplifying is in the present case necessary to get a compact, final expression with `sympy`. A non-expanded `u` might be preferable in other cases - this depends on the problem in question.

The exact solution $u_{\mathrm{e}}(x)$ can be derived by some `sympy` code that closely follows the examples in Section 1.2. The idea is to integrate $-u'' = b$ twice and determine the integration constants from the boundary conditions:

```
C1, C2 = sp.symbols('C1 C2')    # integration constants
f1 = sp.integrate(f, x) + C1
f2 = sp.integrate(f1, x) + C2
# Find C1 and C2 from the boundary conditions u(0)=0, u(1)=1
s = sp.solve([u_e.subs(x,0) - 1, u_e.subs(x,1) - 0], [C1, C2])
# Form the exact solution
u_e = -f2 + s[C1]*x + s[C2]
print 'analytical solution:', u_e
print 'error:', sp.simplify(sp.expand(u - u_e))
```


The last line prints `0`, which is not surprising when $u_{\mathrm{e}}(x)$ is a parabola and our approximate u contains polynomials up to degree 4. It suffices to have $N = 1$, i.e., polynomials of degree 2, to recover the exact solution.

We can play around with the code and test that with $f \sim x^p$, the solution is a polynomial of degree $p+2$, and $N = p+1$ guarantees that the approximate solution is exact.

Although the symbolic code is capable of integrating many choices of $f(x)$, the symbolic expressions for u quickly become lengthy and non-informative, so numerical integration in the code, and hence numerical answers, have the greatest application potential.

6.3 Finite elements

Implementation of the finite element algorithms for differential equations follows closely the algorithm for approximation of functions. The new additional ingredients are

1. other types of integrands (as implied by the variational formulation)
2. additional boundary terms in the variational formulation for Neumann boundary conditions
3. modification of element matrices and vectors due to Dirichlet boundary conditions

Point 1 and 2 can be taken care of by letting the user supply functions defining the integrands and boundary terms on the left- and right-hand side of the equation system:

```
integrand_lhs(phi, r, s, x)
boundary_lhs(phi, r, s, x)
integrand_rhs(phi, r, x)
boundary_rhs(phi, r, x)
```

Here, `phi` is a dictionary where `phi[q]` holds a list of the derivatives of order `q` of the basis functions at the an evaluation point; `r` and `s` are indices for the corresponding entries in the element matrix and vector, and `x` is the global coordinate value corresponding to the current evaluation point.

Given a mesh represented by `vertices`, `cells`, and `dof_map` as explained before, we can write a pseudo Python code to list all the steps in the computational algorithm for finite element solution of a differential equation.

```
<Declare global matrix and rhs: A, b>

for e in range(len(cells)):

    # Compute element matrix and vector
    n = len(dof_map[e])  # no of dofs in this element
    h = vertices[cells[e][1]] - vertices[cells[e][1]]
    <Declare element matrix and vector: A_e, b_e>

    # Integrate over the reference cell
    points, weights = <numerical integration rule>
    for X, w in zip(points, weights):
        phi = <basis functions and derivatives at X>
        detJ = h/2
        x = <affine mapping from X>
        for r in range(n):
            for s in range(n):
                A_e[r,s] += integrand_lhs(phi, r, s, x)*detJ*w
            b_e[r] += integrand_rhs(phi, r, x)*detJ*w
```

```
    # Add boundary terms
    for r in range(n):
        for s in range(n):
            A_e[r,s] += boundary_lhs(phi, r, s, x)*detJ*w
        b_e[r] += boundary_rhs(phi, r, x)*detJ*w

    # Incorporate essential boundary conditions
    for r in range(n):
        global_dof = dof_map[e][r]
        if global_dof in essbc_dofs:
            # dof r is subject to an essential condition
            value = essbc_docs[global_dof]
            # Symmetric modification
            b_e -= value*A_e[:,r]
            A_e[r,:] = 0
            A_e[:,r] = 0
            A_e[r,r] = 1
            b_e[r] = value

    # Assemble
    for r in range(n):
        for s in range(n):
            A[dof_map[e][r], dof_map[e][r]] += A_e[r,s]
        b[dof_map[e][r] += b_e[r]

<solve linear system>
```

7 Variational formulations in 2D and 3D

The major difference between deriving variational formulations in 2D and 3D compared to 1D is the rule for integrating by parts. A typical second-order term in a PDE may be written in dimension-independent notation as

$$\nabla^2 u \quad \text{or} \quad \nabla\cdot(a(\boldsymbol{x})\nabla u)\,.$$

The explicit forms in a 2D problem become

$$\nabla^2 u = \nabla\cdot\nabla u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2},$$

and

$$\nabla\cdot(a(\boldsymbol{x})\nabla u) = \frac{\partial}{\partial x}\left(a(x,y)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(a(x,y)\frac{\partial u}{\partial y}\right)\,.$$

We shall continue with the latter operator as the form arises from just setting $a = 1$.

The general rule for integrating by parts is often referred to as Green's first identity[5]:

$$-\int_\Omega \nabla\cdot(a(\boldsymbol{x})\nabla u)v\,\mathrm{d}x = \int_\Omega a(\boldsymbol{x})\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega} a\frac{\partial u}{\partial n}v\,\mathrm{d}s, \tag{81}$$

where $\partial\Omega$ is the boundary of Ω and $\partial u/\partial n = \boldsymbol{n}\cdot\nabla u$ is the derivative of u in the outward normal direction, $\boldsymbol{n}$ being an outward unit normal to $\partial\Omega$. The integrals $\int_\Omega()\,\mathrm{d}x$ are area integrals in 2D and volume integrals in 3D, while $\int_{\partial\Omega}()\,\mathrm{d}s$ is a line integral in 2D and a surface integral in 3D.

Let us divide the boundary into two parts:

- $\partial\Omega_N$, where we have Neumann conditions $-a\frac{\partial u}{\partial n} = g$, and

[5] http://en.wikipedia.org/wiki/Green's_identities

- $\partial\Omega_D$, where we have Dirichlet conditions $u = u_0$.

The test functions v are required to vanish on $\partial\Omega_D$.

Example. Here is a quite general, stationary, linear PDE arising in many problems:

$$\boldsymbol{v}\cdot\nabla u + \alpha u = \nabla\cdot(a\nabla u) + f, \quad \boldsymbol{x}\in\Omega, \tag{82}$$

$$u = u_0, \quad \boldsymbol{x}\in\partial\Omega_D, \tag{83}$$

$$-a\frac{\partial u}{\partial n} = g, \quad \boldsymbol{x}\in\partial\Omega_N\,. \tag{84}$$

The vector field $\boldsymbol{v}$ and the scalar functions a, α, f, u_0, and g may vary with the spatial coordinate $\boldsymbol{x}$ and must be known.

Such a second-order PDE needs exactly one boundary condition at each point of the boundary, so $\partial\Omega_N\cup\partial\Omega_D$ must be the complete boundary $\partial\Omega$.

Assume that the boundary function $u_0(\boldsymbol{x})$ is defined for all $\boldsymbol{x}\in\Omega$. The unknown function can then be expanded as

$$u = B + \sum_{j\in\mathcal{I}_s} c_j\psi_j, \quad B = u_0\,.$$

The variational formula is obtained from Galerkin's method, which technically implies multiplying the PDE by a test function v and integrating over Ω:

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \alpha u)v\,\mathrm{d}x = \int_\Omega \nabla\cdot(a\nabla u)\,\mathrm{d}x + \int_\Omega fv\,\mathrm{d}x\,.$$

The second-order term is integrated by parts, according to

$$\int_\Omega \nabla\cdot(a\nabla u)\,v\,\mathrm{d}x = -\int_\Omega a\nabla u\cdot\nabla v\,\mathrm{d}x + \int_{\partial\Omega} a\frac{\partial u}{\partial n}v\,\mathrm{d}s\,.$$

The variational form now reads

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \alpha u)v\,\mathrm{d}x = -\int_\Omega a\nabla u\cdot\nabla v\,\mathrm{d}x + \int_{\partial\Omega} a\frac{\partial u}{\partial n}v\,\mathrm{d}s + \int_\Omega fv\,\mathrm{d}x\,.$$

The boundary term can be developed further by noticing that $v\neq 0$ only on $\partial\Omega_N$,

$$\int_{\partial\Omega} a\frac{\partial u}{\partial n}v\,\mathrm{d}s = \int_{\partial\Omega_N} a\frac{\partial u}{\partial n}v\,\mathrm{d}s,$$

and that on $\partial\Omega_N$, we have the condition $a\frac{\partial u}{\partial n} = -g$, so the term becomes

$$-\int_{\partial\Omega_N} gv\,\mathrm{d}s\,.$$

The variational form is then

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \alpha u)v\,\mathrm{d}x = -\int_\Omega a\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega_N} gv\,\mathrm{d}s + \int_\Omega fv\,\mathrm{d}x\,.$$

Instead of using the integral signs we may use the inner product notation:

$$(\boldsymbol{v}\cdot\nabla u, v) + (\alpha u, v) = -(a\nabla u, \nabla v) - (g, v)_N + (f, v)\,.$$

The subscript $_N$ in $(g, v)_N$ is a notation for a line or surface integral over $\partial\Omega_N$.

Inserting the u expansion results in

$$\sum_{j\in\mathcal{I}_s}((\boldsymbol{v}\cdot\nabla\psi_j, \psi_i) + (\alpha\psi_j, \psi_i) + (a\nabla\psi_j, \nabla\psi_i))c_j = (g, \psi_i)_N + (f, \psi_i) - (\boldsymbol{v}\cdot\nabla u_0, \psi_i) + (\alpha u_0, \psi_i) + (a\nabla u_0, \nabla\psi_i)\,.$$

This is a linear system with matrix entries

$$A_{i,j} = (\boldsymbol{v}\cdot\nabla\psi_j, \psi_i) + (\alpha\psi_j, \psi_i) + (a\nabla\psi_j, \nabla\psi_i)$$

and right-hand side entries

$$b_i = (g, \psi_i)_N + (f, \psi_i) - (\boldsymbol{v}\cdot\nabla u_0, \psi_i) + (\alpha u_0, \psi_i) + (a\nabla u_0, \nabla\psi_i),$$

for $i, j \in \mathcal{I}_s$.

In the finite element method, we usually express u_0 in terms of basis functions and restrict i and j to run over the degrees of freedom that are not prescribed as Dirichlet conditions. However, we can also keep all the c_j, $j \in \mathcal{I}_s$, as unknowns drop the u_0 in the expansion for u, and incorporate all the known c_j values in the linear system. This has been explained in detail in the 1D case.

7.1 Transformation to a reference cell in 2D and 3D

We consider an integral of the type

$$\int_{\Omega^{(e)}} a(\boldsymbol{x})\nabla\varphi_i\cdot\nabla\varphi_j\,\mathrm{d}x, \tag{85}$$

where the φ_i functions are finite element basis functions in 2D or 3D, defined in the physical domain. Suppose we want to calculate this integral over a reference cell, denoted by $\tilde{\Omega}^r$, in a coordinate system with coordinates $\boldsymbol{X} = (X_0, X_1)$ (2D) or $\boldsymbol{X} = (X_0, X_1, X_2)$ (3D). The mapping between a point $\boldsymbol{X}$ in the reference coordinate system and the corresponding point $\boldsymbol{x}$ in the physical coordinate system is given by a vector relation $\boldsymbol{x}(\boldsymbol{X})$. The corresponding Jacobian, J, of this mapping has entries

$$J_{i,j} = \frac{\partial x_j}{\partial X_i}\,.$$

The change of variables requires $\mathrm{d}x$ to be replaced by $\det J\,\mathrm{d}X$. The derivatives in the ∇ operator in the variational form are with respect to $\boldsymbol{x}$, which we may denote by $\nabla_{\boldsymbol{x}}$. The $\varphi_i(\boldsymbol{x})$ functions in the integral are replaced by local basis functions $\tilde{\varphi}_r(\boldsymbol{X})$ so the integral features $\nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X})$. We readily have $\nabla_{\boldsymbol{X}}\tilde{\varphi}_r(\boldsymbol{X})$ from formulas for the basis functions in the reference cell, but the desired quantity $\nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X})$ requires some efforts to compute. All the details are provided below.

Let $i = q(e, r)$ and consider two space dimensions. By the chain rule,

$$\frac{\partial\tilde{\varphi}_r}{\partial X} = \frac{\partial\varphi_i}{\partial X} = \frac{\partial\varphi_i}{\partial x}\frac{\partial x}{\partial X} + \frac{\partial\varphi_i}{\partial y}\frac{\partial y}{\partial X},$$

and

$$\frac{\partial\tilde{\varphi}_r}{\partial Y} = \frac{\partial\varphi_i}{\partial Y} = \frac{\partial\varphi_i}{\partial x}\frac{\partial x}{\partial Y} + \frac{\partial\varphi_i}{\partial y}\frac{\partial y}{\partial Y}\,.$$

We can write these two equations as a vector equation

$$\begin{bmatrix} \frac{\partial\tilde{\varphi}_r}{\partial X} \\ \frac{\partial\tilde{\varphi}_r}{\partial Y} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial X} & \frac{\partial y}{\partial X} \\ \frac{\partial x}{\partial Y} & \frac{\partial y}{\partial Y} \end{bmatrix} \begin{bmatrix} \frac{\partial\varphi_i}{\partial x} \\ \frac{\partial\varphi_i}{\partial y} \end{bmatrix}$$

Identifying

$$\nabla_{\boldsymbol{X}}\tilde{\varphi}_r = \begin{bmatrix} \frac{\partial\tilde{\varphi}_r}{\partial X} \\ \frac{\partial\tilde{\varphi}_r}{\partial Y} \end{bmatrix}, \quad J = \begin{bmatrix} \frac{\partial x}{\partial X} & \frac{\partial y}{\partial X} \\ \frac{\partial x}{\partial Y} & \frac{\partial y}{\partial Y} \end{bmatrix}, \quad \nabla_{\boldsymbol{x}}\varphi_r = \begin{bmatrix} \frac{\partial\varphi_i}{\partial x} \\ \frac{\partial\varphi_i}{\partial y} \end{bmatrix},$$

we have the relation

$$\nabla_{\boldsymbol{X}}\tilde{\varphi}_r = J\cdot\nabla_{\boldsymbol{x}}\varphi_i,$$

which we can solve with respect to $\nabla_{\boldsymbol{x}}\varphi_i$:

$$\nabla_{\boldsymbol{x}}\varphi_i = J^{-1}\cdot\nabla_{\boldsymbol{X}}\tilde{\varphi}_r\,. \tag{86}$$

On the reference cell, $\varphi_i(\boldsymbol{x}) = \tilde{\varphi}_r(\boldsymbol{X})$, so

$$\nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X}) = J^{-1}(\boldsymbol{X})\cdot\nabla_{\boldsymbol{X}}\tilde{\varphi}_r(\boldsymbol{X})\,. \tag{87}$$

This means that we have the following transformation of the integral in the physical domain to its counterpart over the reference cell:

$$\int_{\Omega}^{(e)} a(\boldsymbol{x})\nabla_{\boldsymbol{x}}\varphi_i\cdot\nabla_{\boldsymbol{x}}\varphi_j\,\mathrm{d}x\int_{\tilde{\Omega}^r} a(\boldsymbol{x}(\boldsymbol{X}))(J^{-1}\cdot\nabla_{\boldsymbol{X}}\tilde{\varphi}_r)\cdot(J^{-1}\cdot\nabla\tilde{\varphi}_s)\det J\,\mathrm{d}X \tag{88}$$

7.2 Numerical integration

Integrals are normally computed by numerical integration rules. For multi-dimensional cells, various families of rules exist. All of them are similar to what is shown in 1D: $\int f\,\mathrm{d}x \approx \sum_j w_i f(\boldsymbol{x}_j)$, where w_j are weights and $\boldsymbol{x}_j$ are corresponding points.

The file `numint.py`[6] contains the functions `quadrature_for_triangles(n)` and `quadrature_for_tetrahedra` which returns lists of points and weights corresponding to integration rules with `n` points over the reference triangle with vertices $(0,0)$, $(1,0)$, $(0,1)$, and the reference tetrahedron with vertices $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, respectively. For example, the first two rules for integration over a triangle have 1 and 3 points:

```
>>> import numint
>>> x, w = numint.quadrature_for_triangles(num_points=1)
>>> x
[(0.3333333333333333, 0.3333333333333333)]
>>> w
[0.5]
>>> x, w = numint.quadrature_for_triangles(num_points=3)
>>> x
[(0.16666666666666666, 0.16666666666666666),
 (0.66666666666666666, 0.16666666666666666),
 (0.16666666666666666, 0.66666666666666666)]
>>> w
[0.16666666666666666, 0.16666666666666666, 0.16666666666666666]
```

Rules with 1, 3, 4, and 7 points over the triangle will exactly integrate polynomials of degree 1, 2, 3, and 4, respectively. In 3D, rules with 1, 4, 5, and 11 points over the tetrahedron will exactly integrate polynomials of degree 1, 2, 3, and 4, respectively.

[6] `http://tinyurl.com/nm5587k/fem/numint.py`

7.3 Convenient formulas for P1 elements in 2D

We shall now provide some formulas for piecewise linear φ_i functions and their integrals *in the physical coordinate system*. These formulas make it convenient to compute with P1 elements without the need to work in the reference coordinate system and deal with mappings and Jacobians. A lot of computational and algorithmic details are hidden by this approach.

Let $\Omega^{(e)}$ be cell number e, and let the three vertices have global vertex numbers I, J, and K. The corresponding coordinates are (x_I, y_I), (x_J, y_J), and (x_K, y_K). The basis function φ_I over $\Omega^{(e)}$ have the explicit formula

$$\varphi_I(x,y) = \frac{1}{2}\Delta\left(\alpha_I + \beta_I x + \gamma_I y\right), \tag{89}$$

where

$$\alpha_I = x_J y_K - x_K y_J, \tag{90}$$
$$\beta_I = y_J - y_K, \tag{91}$$
$$\gamma_I = x_K - x_J, \tag{92}$$
$$2\Delta = \det \begin{pmatrix} 1 & x_I & y_I \\ 1 & x_J & y_J \\ 1 & x_K & y_K \end{pmatrix}. \tag{93}$$

The quantity Δ is the area of the cell.

The following formula is often convenient when computing element matrices and vectors:

$$\int_{\Omega^{(e)}} \varphi_I^p \varphi_J^q \varphi_K^r dxdy = \frac{p!q!r!}{(p+q+r+2)!} 2\Delta\,. \tag{94}$$

(Note that the q in this formula is not to be mixed with the $q(e,r)$ mapping of degrees of freedom.)

As an example, the element matrix entry $\int_{\Omega^{(e)}} \varphi_I \varphi_J \,\mathrm{d}x$ can be computed by setting $p = q = 1$ and $r = 0$, when $I \neq J$, yielding $\Delta/12$, and $p = 2$ and $q = r = 0$, when $I = J$, resulting in $\Delta/6$. We collect these numbers in a local element matrix:

$$\frac{\Delta}{12}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

The common element matrix entry $\int_{\Omega^{(e)}} \nabla\varphi_I \cdot \nabla\varphi_J \,\mathrm{d}x$, arising from a Laplace term $\nabla^2 u$, can also easily be computed by the formulas above. We have

$$\nabla\varphi_I \cdot \nabla\varphi_J = \frac{\Delta^2}{4}(\beta_I\beta_J + \gamma_I\gamma_J) = \text{const},$$

so that the element matrix entry becomes $\frac{1}{4}\Delta^3(\beta_I\beta_J + \gamma_I\gamma_J)$.

From an implementational point of view, one will work with local vertex numbers $r = 0, 1, 2$, parameterize the coefficients in the basis functions by r, and look up vertex coordinates through $q(e,r)$.

Similar formulas exist for integration of P1 elements in 3D.

8 Summary

- When approximating f by $u = \sum_j c_j\varphi_j$, the least squares method and the Galerkin/projection method give the same result. The interpolation/collocation method is simpler and yields different (mostly inferior) results.
- Fourier series expansion can be viewed as a least squares or Galerkin approximation procedure with sine and cosine functions.
- Basis functions should optimally be orthogonal or almost orthogonal, because this gives little round-off errors when solving the linear system, and the coefficient matrix becomes diagonal or sparse.
- Finite element basis functions are *piecewise* polynomials, normally with discontinuous derivatives at the cell boundaries. The basis functions overlap very little, leading to stable numerics and sparse matrices.
- To use the finite element method for differential equations, we use the Galerkin method or the method of weighted residuals to arrive at a variational form. Technically, the differential equation is multiplied by a test function and integrated over the domain. Second-order derivatives are integrated by parts to allow for typical finite element basis functions that have discontinuous derivatives.
- The least squares method is not much used for finite element solution of differential equations of second order, because it then involves second-order derivatives which cause trouble for basis functions with discontinuous derivatives.
- We have worked with two common finite element terminologies and associated data structures (both are much used, especially the first one, while the other is more general):
  1. *elements*, *nodes*, and *mapping between local and global node numbers*
  2. an extended element concept consisting of *cell*, *vertices*, *degrees of freedom*, *local basis functions*, *geometry mapping*, and *mapping between local and global degrees of freedom*
- The meaning of the word "element" is multi-fold: the geometry of a finite element (also known as a cell), the geometry and its basis functions, or all information listed under point 2 above.
- One normally computes integrals in the finite element method element by element (cell by cell), either in a local reference coordinate system or directly in the physical domain.
- The advantage of working in the reference coordinate system is that the mathematical expressions for the basis functions depend on the element type only, not the geometry of that element in the physical domain. The disadvantage is that a mapping must be used, and derivatives must be transformed from reference to physical coordinates.
- Element contributions to the global linear system are collected in an element matrix and vector, which must be assembled into the global system using the degree of freedom mapping (`dof_map`) or the node numbering mapping (`elements`), depending on which terminology that is used.

- Dirichlet conditions, involving prescribed values of u at the boundary, are implemented either via a boundary function that take on the right Dirichlet values, while the basis functions vanish at such boundaries. In the finite element method, one has a general expression for the boundary function, but one can also incorporate Dirichlet conditions in the element matrix and vector or in the global matrix system.
- Neumann conditions, involving prescribed values of the derivative (or flux) of u, are incorporated in boundary terms arising from integrating terms with second-order derivatives by part. Forgetting to account for the boundary terms implies the condition $\partial u/\partial n = 0$ at parts of the boundary where no Dirichlet condition is set.

9 Exercises

Exercise 1: Refactor functions into a more general class

Section 1.2 displays three functions for computing the analytical solution of some simple model problems. There is quite some repetitive code, suggesting that the functions can benefit from being refactored into a class where the user can define the $f(x)$, $a(x)$, and the boundary conditions in particular methods in subclasses. Demonstrate how the new class can be used to solve the three particular problems in Section 1.2.

In the method that computes the solution, check that the solution found fulfills the differential equation and the boundary conditions. Filename: `uxx_f_sympy_class.py`.

Exercise 2: Compute the deflection of a cable with sine functions

A hanging cable of length L with significant tension T has a downward deflection $w(x)$ governed by

Solve

$$Tw''(x) = \ell(x),$$

when $\ell(x)$ the vertical load per unit length. The cable is fixed at $x = 0$ and $x = L$ so the boundary conditions become $w(0) = w(L) = 0$.

If we assume a constant load $\ell(x) = \text{const}$, the solution is expected to be symmetric around $x = L/2$. For a function $w(x)$ that is symmetric around some point x_0, it means that $w(x_0 - h) = w(x_0 + h)$, and then $w'(x_0) = \lim_{h\to 0}(w(x_0 + h) - w(x_0 - h))/(2h) = 0$. We can therefore halve the domain and seek $w(x)$ in $[0, L/2]$ with boundary conditions $w(0) = 0$ and $w'(L/2) = 0$.

The problem can be scaled by introducing a dimensionless coordinate (also called x) in $[0, 1]$ and a dimensionless vertical deflection $u(x)$. The differential equation problem for $u(x)$ becomes

$$u'' = 1, \quad x \in (0,1), \quad u(0) = 0,\ u'(1) = 0\,.$$

A possible function space is spanned by $\psi_i = \sin((2i+1)\pi x/2)$, $i = 0, \ldots, N$. Use a Galerkin and a least squares method to find the coefficients c_j in $u(x) = \sum_j c_j\psi_j$. Find how fast the coefficients decrease in magnitude by looking at c_j/c_{j-1}. Find the error in the maximum deflection at $x = 1$ when only one basis function is used ($N = 0$).

What happens if we choose basis functions $\psi_i = \sin((i+1)\pi x)$? These basis functions are appropriate if we do not utilize symmetry and solve the original problem on $[0, L]$. A scaled version of this problem reads

$$u'' = 1, \quad x \in (0,1), \quad u(0) = u(1) = 0\,.$$

Carry out the computations with $N = 0$ and demonstrate that the maximum deflection $u(1/2)$ is the same in the problem utilizing symmetry and the problem covering the whole cable. Filenames: `cable_sin.pdf`, `cable_sin.py`.

Exercise 3: Check integration by parts

Consider the Galerkin method for the problem involving u in Exercise 2. Show that the formulas for c_j are independent of whether we perform integration by parts or not. Filename: `cable_integr_by_parts.pdf`.

Exercise 4: Compute the deflection of a cable with 2 P1 elements

Solve the problem for u in Exercise 2 using two P1 linear elements. Filename: `cable_2P1.pdf`.

Exercise 5: Compute the deflection of a cable with 1 P2 element

Solve the problem for u in Exercise 2 using one P2 element with quadratic basis functions. Filename: `cable_1P2.pdf`.

Exercise 6: Compute the deflection of a cable with a step load

We consider the deflection of a tension cable as described in Exercise 2. Now the load is

$$\ell(x) = \begin{cases} \ell_1, & x < L/2, \\ \ell_2, & x \geq L/2 \end{cases} \qquad x \in [0, L]\,.$$

This load is not symmetric with respect to the midpoint $x = L/2$ so the solution loses its symmetry and we must solve the scaled problem

$$u'' = \begin{cases} 1, & x < 1/2, \\ 0, & x \geq 1/2 \end{cases} \qquad x \in (0,1), \quad u(0) = 0,\ u(1) = 0\,.$$

a) Use $\psi_i = \sin((i+1)\pi x)$, $i = 0, \ldots, N$ and the Galerkin method without integration by parts. Derive a formula for c_j in the solution expansion $u = \sum_j c_j\psi_j$. Plot how fast the coefficients c_j tend to zero (on a log scale).

b) Solve the problem with P1 finite elements. Plot the solution for $N_e = 2, 4, 8$ elements. Filename: `cable_discont_load.pdf`.

Exercise 7: Show equivalence between linear systems

Incorporation of Dirichlet conditions at $x = 0$ and $x = L$ in a finite element mesh on $\Omega = [0, L]$ can either be done by introducing an expansion $u(x) = U_0\varphi_0 + U_{N_n-1}\varphi_{N_n-1} + \sum_{j=0}^{N} c_j\varphi_{\nu(j)}$, with $N = N_n - 3$ and considering u values at the inner nodes as unknowns, *or* one can assemble the matrix system with $u(x) = \sum_{j=0}^{N=N_n-1} c_j\varphi_j$ and afterwards replace the rows corresponding to known c_j values by the boundary conditions. Show that the two approaches are equivalent.

Exercise 8: Compute with a non-uniform mesh

Derive the linear system for the problem $-u'' = 2$ on $[0,1]$, with $u(0) = 0$ and $u(1) = 1$, using P1 elements and a *non-uniform* mesh. The vertices have coordinates $x_0 = 0 < x_1 < \cdots < x_{N_n-1} = 1$, and the length of cell number e is $h_e = x_{e+1} - x_e$.

It is of interest to compare the discrete equations for the finite element method in a non-uniform mesh with the corresponding discrete equations arising from a finite difference method. Go through the derivation of the finite difference formula $u''(x_i) \approx [D_x D_x u]_i$ and modify it to find a natural discretization of $u''(x_i)$ on a non-uniform mesh. Filename: `nonuniform_P1.pdf`.

Problem 9: Solve a 1D finite element problem by hand

The following scaled 1D problem is a very simple, yet relevant, model for convective transport in fluids:

$$u' = \epsilon u'', \quad u(0) = 0,\ u(1) = 1,\ x \in [0,1]\,. \tag{95}$$

a) Find the analytical solution to this problem. (Introduce $w = u'$, solve the first-order differential equation for $w(x)$, and integrate once more.)

b) Derive the variational form of this problem.

c) Introduce a finite element mesh with uniform partitioning. Use P1 elements and compute the element matrix and vector for a general element.

d) Incorporate the boundary conditions and assemble the element contributions.

e) Identify the resulting linear system as a finite difference discretization of the differential equation using

$$[D_{2x} u = \epsilon D_x D_x u]_i\,.$$

f) Compute the numerical solution and plot it together with the exact solution for a mesh with 20 elements and $\epsilon = 10, 1, 0.1, 0.01$.
Filename: `convdiff1D_P1.pdf`.

Exercise 10: Compare finite elements and differences for a radially symmetric Poisson equation

We consider the Poisson problem in a disk with radius R with Dirichlet conditions at the boundary. Given that the solution is radially symmetric and hence dependent only on the radial coordinate ($r = \sqrt{x^2 + y^2}$), we can reduce the problem to a 1D Poisson equation

$$-\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) = f(r), \quad r \in (0,R),\ u'(0) = 0,\ u(R) = U_R\,. \tag{96}$$

a) Derive a variational form of (96) by integrating over the whole disk, or posed equivalently: use a weighting function $2\pi r v(r)$ and integrate r from 0 to R.

b) Use a uniform mesh partition with P1 elements and show what the resulting set of equations becomes. Integrate the matrix entries exact by hand, but use a Trapezoidal rule to integrate the f term.

c) Explain that an intuitive finite difference method applied to (96) gives

$$\frac{1}{r_i}\frac{1}{h^2}\left(r_{i+\frac{1}{2}}(u_{i+1} - u_i) - r_{i-\frac{1}{2}}(u_i - u_{i-1})\right) = f_i, \quad i = rh\,.$$

For $i = 0$ the factor $1/r_i$ seemingly becomes problematic. One must always have $u'(0) = 0$, because of the radial symmetry, which implies $u_{-1} = u_1$, if we allow introduction of a fictitious value u_{-1}. Using this u_{-1} in the difference equation for $i = 0$ gives

$$\frac{1}{r_0}\frac{1}{h^2}\left(r_{\frac{1}{2}}(u_1 - u_0) - r_{-\frac{1}{2}}(u_0 - u_1)\right) = \frac{1}{r_0}\frac{1}{2h^2}\left((r_0 + r_1)(u_1 - u_0) - (r_{-1} + r_0)(u_0 - u_1)\right) \approx 2(u_1 - u_0),$$

if we use $r_{-1} + r_1 \approx 2r_0$.

Set up the complete set of equations for the finite difference method and compare to the finite element method in case a Trapezoidal rule is used to integrate the f term in the latter method. Filename: `radial_Poisson1D_P1.pdf`.

Exercise 11: Compute with variable coefficients and P1 elements by hand

Consider the problem

$$-\frac{d}{dx}\left(a(x)\frac{du}{dx}\right) + \gamma u = f(x), \quad x \in \Omega = [0,L], \quad u(0) = \alpha,\ u'(L) = \beta\,. \tag{97}$$

We choose $a(x) = 1 + x^2$. Then

$$u(x) = \alpha + \beta(1 + L^2)\tan^{-1}(x), \tag{98}$$

is an exact solution if $f(x) = \gamma u$.

Derive a variational formulation and compute general expressions for the element matrix and vector in an arbitrary element, using P1 elements and a uniform partitioning of $[0,L]$. The right-hand side integral is challenging and can be computed by a numerical integration rule. The Trapezoidal rule (**??**) gives particularly simple expressions. Filename: `atan1D_P1.pdf`.

Exercise 12: Solve a 2D Poisson equation using polynomials and sines

The classical problem of applying a torque to the ends of a rod can be modeled by a Poisson equation defined in the cross section Ω:

$$-\nabla^2 u = 2, \quad (x,y) \in \Omega,$$

with $u = 0$ on $\partial\Omega$. Exactly the same problem arises for the deflection of a membrane with shape Ω under a constant load.

For a circular cross section one can readily find an analytical solution. For a rectangular cross section the analytical approach ends up with a sine series. The idea in this exercise is to use a single basis function to obtain an approximate answer.

We assume for simplicity that the cross section is the unit square: $\Omega = [0,1] \times [0,1]$.

a) We consider the basis $\psi_{p,q}(x,y) = \sin((p+1)\pi x)\sin(q\pi y)$, $p,q = 0,\ldots,n$. These basis functions fulfill the Dirichlet condition. Use a Galerkin method and $n = 0$.

b) The basis function involving sine functions are orthogonal. Use this property in the Galerkin method to derive the coefficients $c_{p,q}$ in a formula $u = \sum_p \sum_q c_{p,q}\psi_{p,q}(x,y)$.

c) Another possible basis is $\psi_i(x,y) = (x(1-x)y(1-y))^{i+1}$, $i = 0,\ldots,N$. Use the Galerkin method to compute the solution for $N = 0$. Which choice of a single basis function is best, $u \sim x(1-x)y(1-y)$ or $u \sim \sin(\pi x)\sin(\pi y)$? In order to answer the question, it is necessary to search the web or the literature for an accurate estimate of the maximum u value at $x = y = 1/2$. Filename: `torsion_sin_xy.pdf`.

References

[1] H. P. Langtangen. Approximation of functions. *http://tinyurl.com/k3sdbuv/pub*.

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